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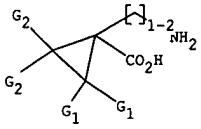

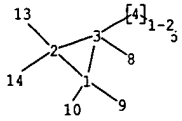

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4 5 8 9 10 13 14
ring nodes :
1 2 3
chain bonds :
1-9 1-10 2-13 2-14 3-4 3-8 4-5
ring bonds :
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exact/norm bonds :
1-2 1-3 1-9 1-10 2-3 2-13 2-14 4-5
exact bonds :
3-4 3-8

G1:H,CH3,Et

G2:C,H,Ph,Cb,Ak,O

Match level :
1:Atom 2:Atom 3:Atom 4:CLASS 5:CLASS 8:CLASS 9:CLASS 10:CLASS 13:CLASS 14:CLASS

10760032-R3 AND R4 NON CICLYC

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
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NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 26	CA/CAPLUS - Expanded patent coverage to include the Russian Agency for Patents and Trademarks (ROSPATENT)
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

10760032-R3 AND R4 NON CICLYC

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=> file registry
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 9 FEB 2005 HIGHEST RN 828241-21-0
DICTIONARY FILE UPDATES: 9 FEB 2005 HIGHEST RN 828241-21-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L1 STRUCTURE UPLOADED

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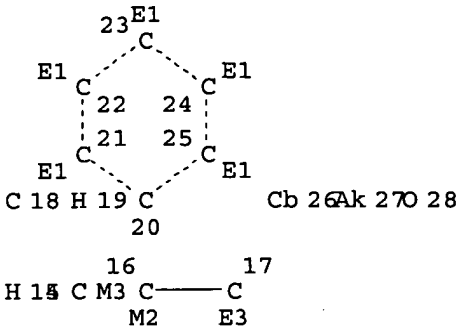
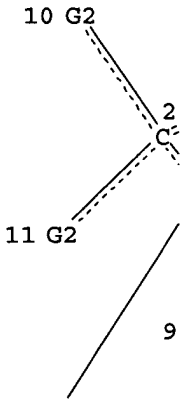
L1 HAS NO ANSWERS
L1 STR

10760032-R3 AND R4 NON CICLYC





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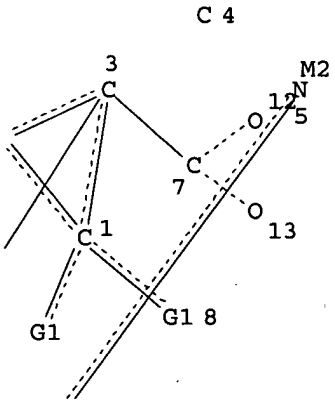

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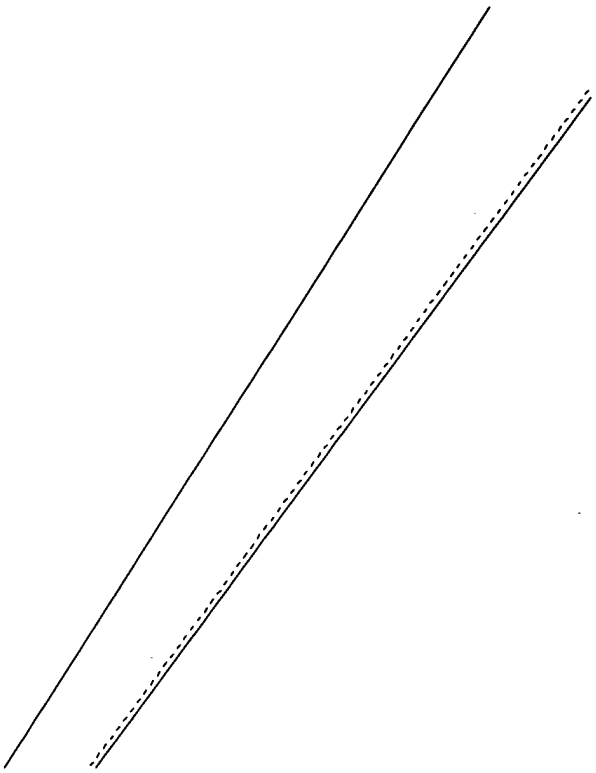
10760032-R3 AND R4 NON CICLYC



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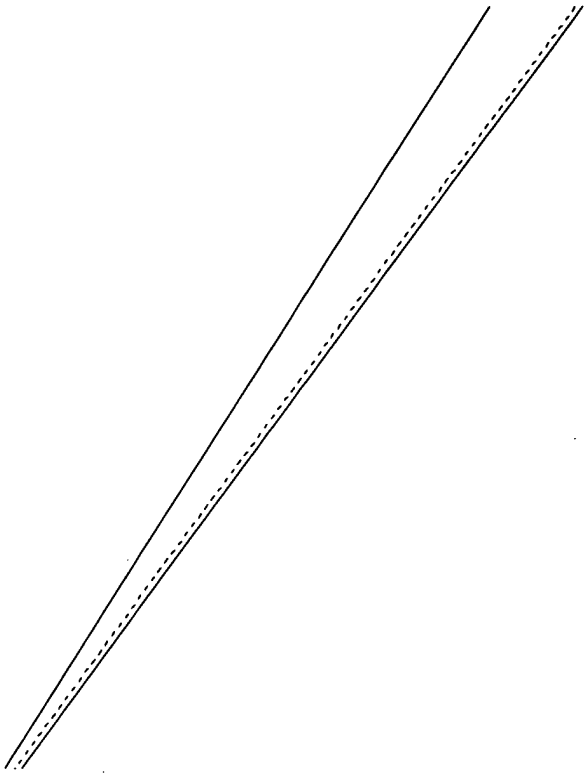
10760032-R3 AND R4 NON CICLYC



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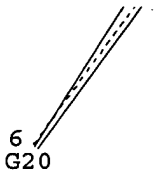

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HCOUNT IS E1 AT 24
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10760032-R3 AND R4 NON CICLYC

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MLEVEL IS CLASS AT 4 5 7 12 13 14 15 16 17 18 19 20 21 22 23 24 25
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

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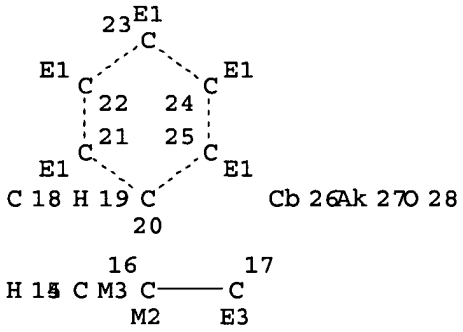
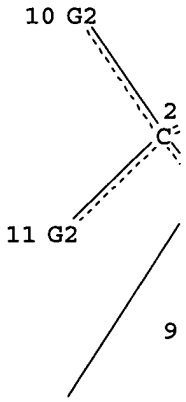
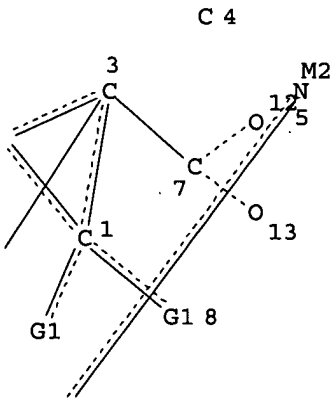
L1 STR







10760032-R3 AND R4 NON CICLYC

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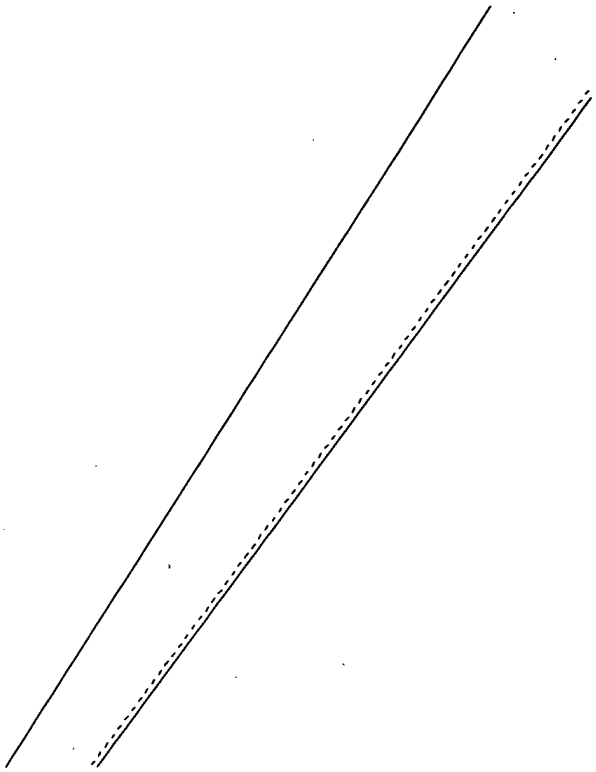

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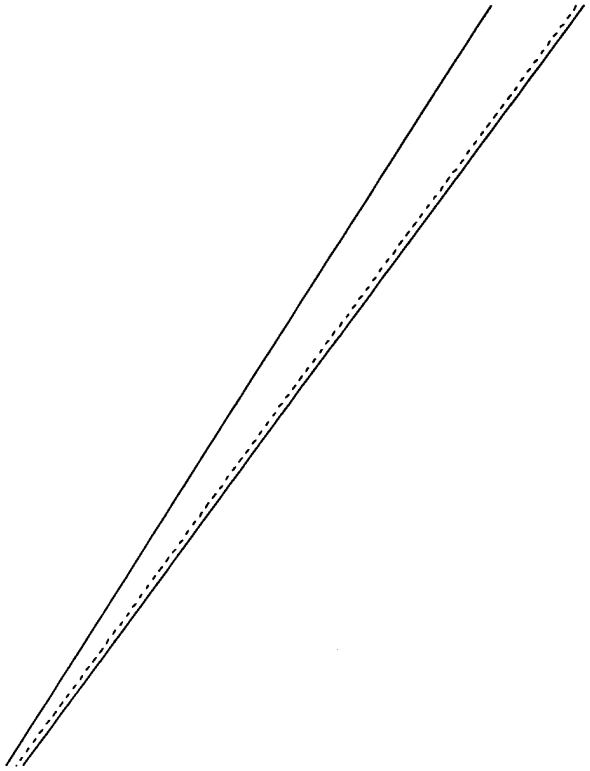

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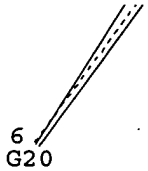

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G20

Page 4-A
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10760032-R3 AND R4 NON CICLYC

NSPEC IS C AT 11
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DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 4 5 7 12 13 14 15 16 17 18 19 20 21 22 23 24 25
26 27 28
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

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FULL SCREEN SEARCH COMPLETED - 5239 TO ITERATE

100.0% PROCESSED 5239 ITERATIONS 65 ANSWERS
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FULL ESTIMATED COST 162.19 162.40

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FILE COVERS 1907 - 11 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 9 Feb 2005 (20050209/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2 full
L3 38 L2

=> d 1-38 bib abs hitstr l3

L3 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:756699 CAPLUS
DN 141:277627
TI Preparation of tetrazole and oxadiazolone substituted β-amino acid derivatives as ligands of the α2δ-subunit of a calcium channel

10760032-R3 AND R4 NON CICLYC

IN Barta, Nancy Sue; Colbry, Norman Lloyd; Hudack, Raymond Andrew, Jr.; Lin, Kristin Knapp; Schwarz, Jacob Bradley; Thorpe, Andrew John; Wustrow, David Juergen; Zhu, Zhijian
PA Warner-Lambert Company LLC, USA
SO PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004078734	A1	20040916	WO 2004-IB510	20040223
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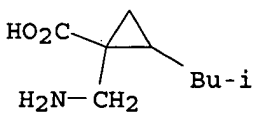
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2005014804	A1	20050120	US 2004-795760	20040308
PRAI	US 2003-452871P	P	20030307		

OS MARPAT 141:277627

AB Title compds. R2R1(NH2)C-C(G)R3R4 [G = tetrazolyl, 1,3,5-oxadiazol-2-one; R1-2 = H, alkyl, alkoxy, etc.; R3-4 = H, Me; (I)] and related cyclopropane derivs. are prepared For instance, 4-methyl-2-(1H-tetrazol-5-yl)pentylamine is prepared from 1-benzyl-1H-tetrazole and 4-methyl-1-nitropentene in 2 steps. Selected example compds. exhibit binding with nM to μM affinity for α2δ-subunit of the calcium channel (3 biol. examples). I are useful for the treatment of central nervous system and other disorders.

IT **724772-89-8P 724772-90-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tetrazole and oxadiazolone substituted β-amino acid derivs. as ligands of α2δ-subunit of a calcium channel for use as CNS agents)

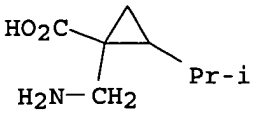
RN 724772-89-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 724772-90-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

10760032-R3 AND R4 NON CICLYC



● HCl

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:633436 CAPLUS
DN 141:174191
TI Preparation of pyrazolopyrimidines as a small conductance potassium channel (SK channel) blocking agents
IN Takamuro, Iwao; Sekine, Yasuo; Tsuboi, Yasunori; Nogi, Kouji; Taniguchi, Hiroyuki
PA Tanabe Seiyaku Co., Ltd., Japan
SO PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004064721	A2	20040805	WO 2004-JP617	20040123
	WO 2004064721	A3	20040923		

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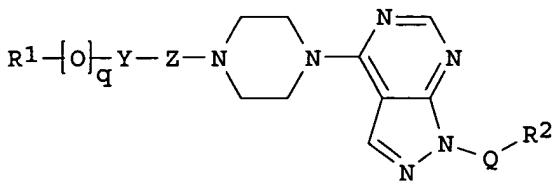
PRAI	JP 2003-16770	A	20030124
	JP 2003-205341	A	20030801
	JP 2003-385399	A	20031114

OS MARPAT 141:174191
GI

10760032-R3 AND R4 NON CICLYC



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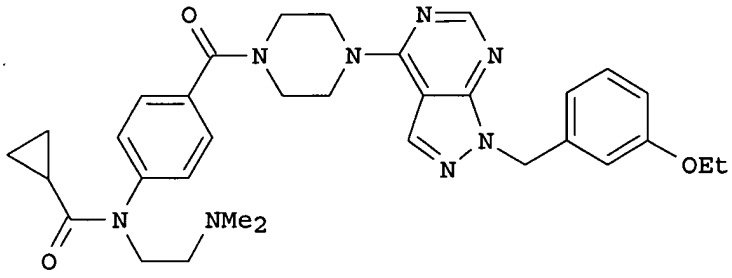


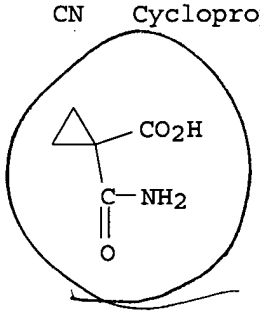
II

AB The title compds. [I; R1 = substituted aryl, (un)substituted nitrogen-containing aliphatic heteromonocyclyl, substituted cycloalkyl, (un)substituted amino, or substituted heteroaryl; R2 = (un)substituted (hetero)aryl; Y = a single bond, alkylene or alkenylene; Z = CO, CH2, S02, C:N(CN); Q = alkylene; q = 0-1] and their pharmaceutically acceptable salts, which have a small conductance potassium channel (SK channel) blocking activity, were prepared Thus, treating Et 4-{N-(cyclopropylcarbonyl)-N-[2-(dimethylamino)ethyl]amino}benzoate (preparation given) with 2N NaOH solution followed by treatment with 2N HCl, and the reaction of the resulting acid with 1-(3-ethoxybenzyl)-4-(piperazin-1-yl)-1H-pyrazol[3,4-d]pyrimidine dihydrochloride afforded 84% II which showed an excellent apamin-binding inhibitory activity (IC50 of 0.05 μM). The pharmaceutical composition comprising the compound I is claimed.

IT **6914-74-5**, 1-Carbamoyl-1-cyclopropanecarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolopyrimidines as a small conductance potassium channel (SK channel) blocking agents)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



MW ≠ C

L3 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:612495 CAPLUS

DN 141:123903

TI Preparation of cyclopropyl β-amino acid derivatives for pharmaceutical use

IN Schwarz, Jacob Bradley; Wustrow, David Juergen

PA ~~USA~~

SO U.S. Pat. Appl. Publ., 22 pp.
CODEN: USXXCO

Jane Inventors

10760032-R3 AND R4 NON CICLYC

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004147608	A1	20040729	US 2004-760032	20040116
	WO 2004065361	A2	20040805	WO 2004-IB58	20040109
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PRAI US 2003-441825P P 20030122
OS MARPAT 141:123903
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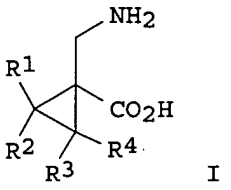


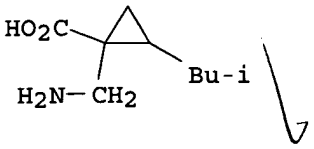
I

AB The invention relates to novel cyclopropyl β-amino acids derivs. I [R1 and R2 are H, alkyl, alkoxyalkyl, phenylalkyl or phenylalkoxyalkyl, where the Ph moieties can optionally be substituted with one or two halo or alkyl groups; or R1R2C is cyclopentyl, cyclohexyl or cycloheptyl which can be substituted with one or two groups R1/R2; R3, R4 are H or Me] and pharmaceutical compns. containing them for use in the treatment of central nervous system and other disorders. Compds. I exhibit activity as α2δ ligands and have affinity for the α2δ subunit of a calcium channel. Thus, 1-aminomethylspiro[2.5]octane-1-carboxylic acid hydrochloride was prepared by treating cyanocyclohexylideneacetic acid Et ester with nitromethane in MeCN in the presence of DBU, followed by hydrogenation over Raney Ni and hydrolysis with 3N HCl.

IT **724772-89-8P 724772-90-1P 724772-91-2P**
724772-93-4P 724772-94-5P 724772-95-6P
724772-96-7P 724772-99-0P 724773-00-6P
724773-01-7P 724773-08-4P 724773-09-5P
724773-10-8P 724773-11-9P 724773-12-0P
724773-13-1P 724773-14-2P 724773-15-3P
724773-16-4P 724773-17-5P 724773-18-6P
724773-19-7P 724773-20-0P 724773-21-1P
724773-22-2P 724773-23-3P 724773-24-4P
724773-26-6P 724773-28-8P 724773-30-2P
724773-31-3P 724773-32-4P 724773-34-6P
724773-36-8P 724773-37-9P 724773-38-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopropyl β-amino acid derivs. for pharmaceutical use)

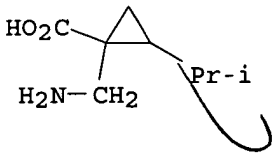
RN 724772-89-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

10760032-R3 AND R4 NON CICLYC



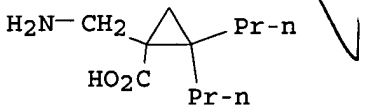
● HCl

RN 724772-90-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

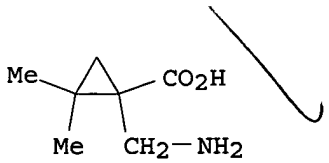


● HCl

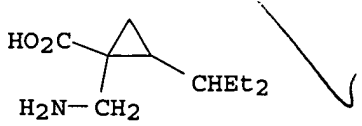
RN 724772-91-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2,2-dipropyl- (9CI) (CA INDEX NAME)



RN 724772-93-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2,2-dimethyl- (9CI) (CA INDEX NAME)

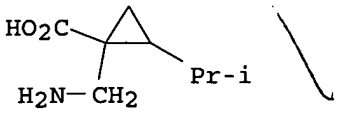


RN 724772-94-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(1-ethylpropyl)- (9CI) (CA INDEX NAME)

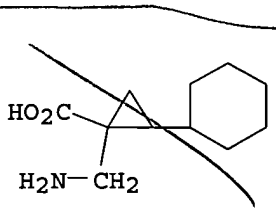


RN 724772-95-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(1-methylethyl)- (9CI) (CA

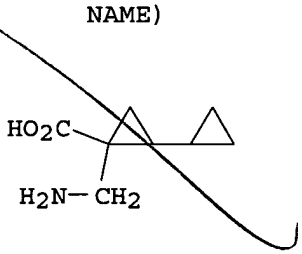
INDEX NAME)



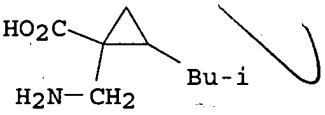
RN 724772-96-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-cyclohexyl- (9CI) (CA INDEX NAME)



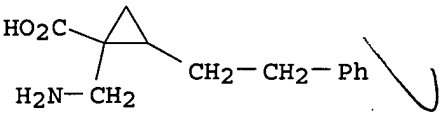
RN 724772-99-0 CAPLUS
CN [1,1'-Bicyclopropyl]-2-carboxylic acid, 2-(aminomethyl)- (9CI) (CA INDEX NAME)



RN 724773-00-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

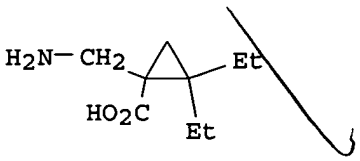


RN 724773-01-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-phenylethyl)- (9CI) (CA INDEX NAME)

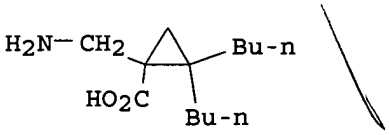


RN 724773-08-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2,2-diethyl- (9CI) (CA INDEX NAME)

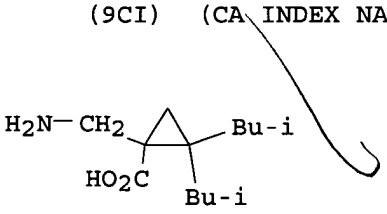
10760032-R3 AND R4 NON CICLYC



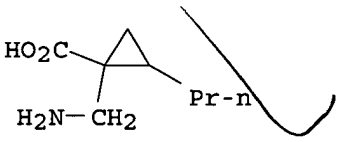
RN 724773-09-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2,2-dibutyl- (9CI) (CA INDEX NAME)



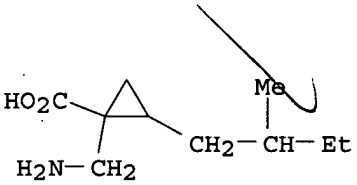
RN 724773-10-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2,2-bis(2-methylpropyl)- (9CI) (CA INDEX NAME)



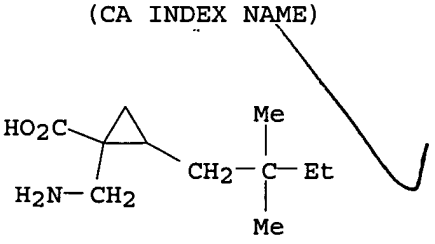
RN 724773-11-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-propyl- (9CI) (CA INDEX NAME)



RN 724773-12-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-methylbutyl)- (9CI) (CA INDEX NAME)

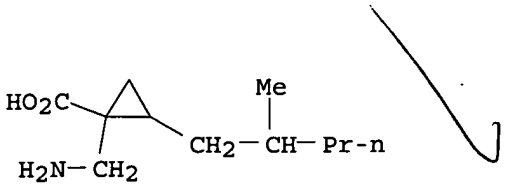


RN 724773-13-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2,2-dimethylbutyl)- (9CI) (CA INDEX NAME)

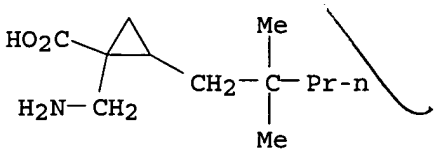


10760032-R3 AND R4 NON CICLYC

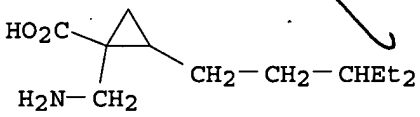
RN 724773-14-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-methylpentyl)- (9CI) (CA INDEX NAME)



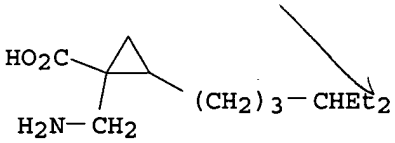
RN 724773-15-3 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2,2-dimethylpentyl)- (9CI) (CA INDEX NAME)



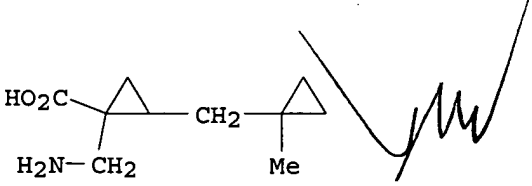
RN 724773-16-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(3-ethylpentyl)- (9CI) (CA INDEX NAME)



RN 724773-17-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(4-ethylhexyl)- (9CI) (CA INDEX NAME)

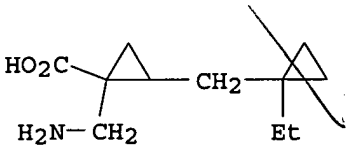


RN 724773-18-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-[(1-methylcyclopropyl)methyl]- (9CI) (CA INDEX NAME)

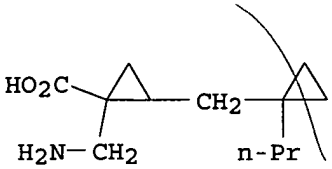


RN 724773-19-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-[(1-ethylcyclopropyl)methyl]- (9CI) (CA INDEX NAME)

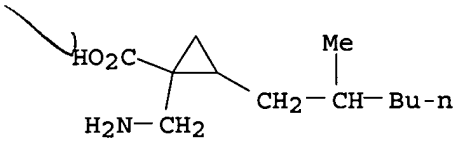
10760032-R3 AND R4 NON CICLYC



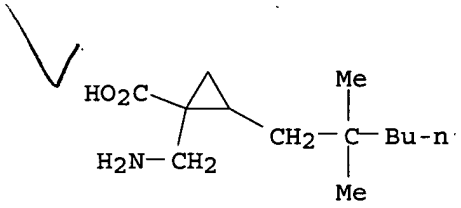
RN 724773-20-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-[(1-propylcyclopropyl)methyl]- (9CI) (CA INDEX NAME)



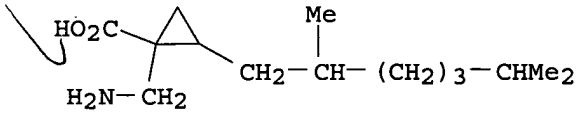
RN 724773-21-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-methylhexyl)- (9CI) (CA INDEX NAME)



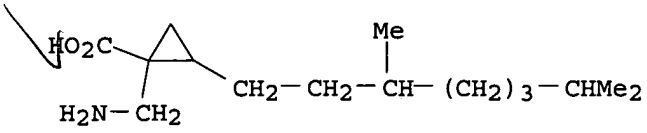
RN 724773-22-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2,2-dimethylhexyl)- (9CI) (CA INDEX NAME)



RN 724773-23-3 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2,6-dimethylheptyl)- (9CI) (CA INDEX NAME)

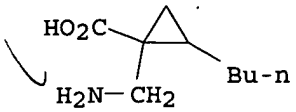


RN 724773-24-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(3,7-dimethyloctyl)- (9CI) (CA INDEX NAME)

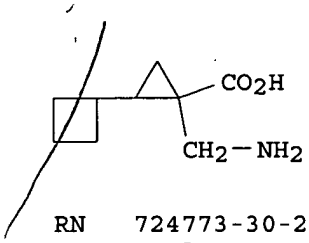


10760032-R3 AND R4 NON CICLYC

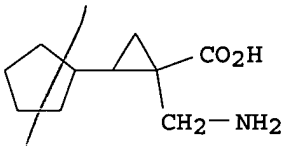
RN 724773-26-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-butyl- (9CI) (CA INDEX NAME)



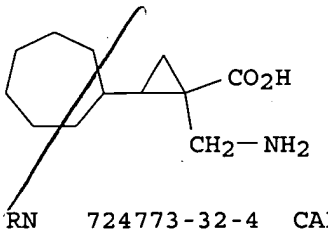
RN 724773-28-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-cyclobutyl- (9CI) (CA INDEX NAME)



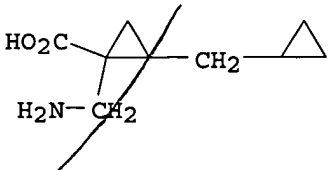
RN 724773-30-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-cyclopentyl- (9CI) (CA INDEX NAME)



RN 724773-31-3 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-cycloheptyl- (9CI) (CA INDEX NAME)

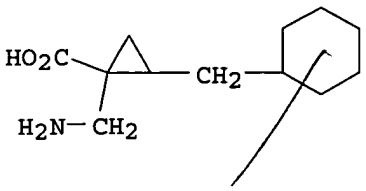


RN 724773-32-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(cyclopropylmethyl)- (9CI) (CA INDEX NAME)

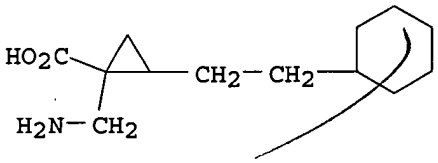


RN 724773-34-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(cyclohexylmethyl)- (9CI) (CA INDEX NAME)

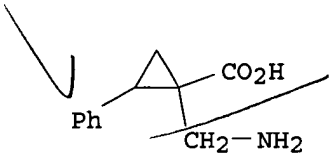
10760032-R3 AND R4 NON CICLYC



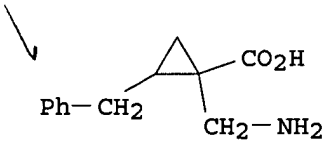
RN 724773-36-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(2-cyclohexylethyl)- (9CI) (CA INDEX NAME)



RN 724773-37-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 724773-38-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:534173 CAPLUS
DN 141:89016
TI Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection
IN Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph; Bifulco, Neil; Boros, Eric Eugene; Chauder, Brian Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; Mclean, Ed Williams; Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin; Vanderwall, Dana
PA Smithkline Beecham Corporation, USA; et al.
SO PCT Int. Appl., 859 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004054974	A2	20040701	WO 2003-US39644	20031212
	WO 2004054974	A3	20040902		

10760032-R3 AND R4 NON CICLYC

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-433634P P 20021213
OS MARPAT 141:89016
GI

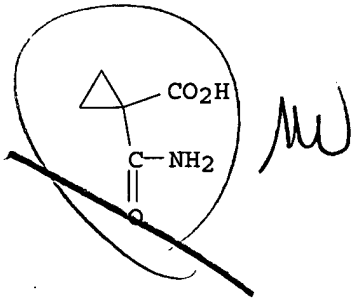
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl, carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl, heteroarylcycloalkyl, aralkylcarbonyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thioxo groups or halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoimino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocarbonyl, oxyiminomethyl, thioiminomethyl, amino(cyanoimino)methyl, (cyanoimino)methyl, amino(acylimino)methyl, amino(sulfonylimino)methyl, amino(sulfinylimino)methyl, amino(alkoxyimino)methyl, amino(imino)methyl, (cyanoimino)methoxy, iminomethoxy, (cyanoimino)methanethiyl, alkylcarbonyloxy; A = saturated, partially saturated, or aromatic monocyclic ring with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5 nitrogen, oxygen, and/or sulfur atoms] such as II are prepared I are prepared as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention compds. have pIC50 values of ≥5 in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepared in four steps from 4-phenyl-4-piperidinecarbonitrile by protection of the piperidine with Boc anhydride, reduction of the nitrile with diisobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepared in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduction of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxyborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II.

IT **6914-74-5**, 1-(Aminocarbonyl)-1-cyclopropanecarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of benzimidazolylazabicyclooctylethylpiperidine Ccr5 antagonists in the treatment of bacterial and viral infections

10760032-R3 AND R4 NON CICLYC

and other diseases)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)

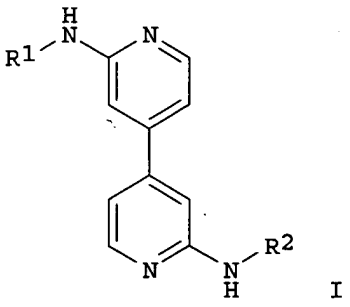


L3 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:515503 CAPLUS
DN 141:71452
TI Preparation of pyridine derivatives as JNK inhibitors
IN Kallin, Elisabeth; Plobeck, Niklas; Swahn, Britt-Marie
PA Astrazeneca Ab, Swed.
SO PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004052880	A1	20040624	WO 2003-SE1911	20031208

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI SE 2002-3654 A 20021209
OS MARPAT 141:71452
GI



I

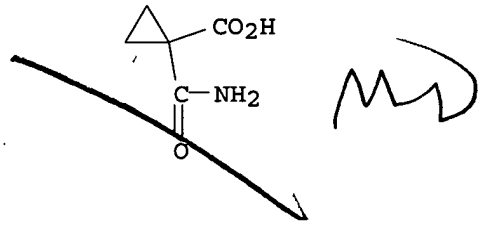
AB The title compds. [I; R1 = aryl or heteroaryl, each of which is optionally substituted with one or more of R3, OR3, OCOR3, COOR3, COR3, CONR3R4, NHCOR3, NR3R4, NHSO2R3, SO2R3, SO2NR3R4, SR3, CN, halo, NO2; R2 = R5, R6, COR5, COR6, CONHR5, CONHR6, CON(R6)2, COOR5, COOR6, SO2R5, SO2R6; R3, R4 = H, alkyl, cycloalkyl, etc.; R5 = (un)substituted (hetero)aryl; R6 = H,

alkyl, cycloalkyl, etc.], were prepared and formulated. E.g., a 4-step synthesis of N,N'-bis[4-(trifluoromethyl)phenyl]-4,4'-bipyridine-2,2'-diamine, starting from 2-chloropyridine, was given. Typical Ki values for the compds. I are in the range of about 0.001 to about 10,000 nM in assay for inhibition of JNK3.

IT **6914-74-5**, 1-(Aminocarbonyl)cyclopropanecarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4,4-bipyridine-2,2'-diamine derivs. as JNK inhibitors)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:972059 CAPLUS

DN 140:27819

TI Preparation of pyrazole derivatives as JNK inhibitors

IN Ohi, Norihito; Sato, Nobuaki; Soejima, Motohiro; Doko, Takashi; Terauchi, Taro; Naoe, Yoshimitsu; Motoki, Takafumi

PA Eisai Co., Ltd., Japan

SO PCT Int. Appl., 561 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003101968	A1	20031211	WO 2003-JP6777	20030529

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

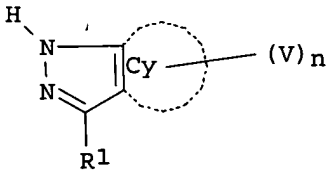
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI JP 2002-158467 A 20020531

JP 2003-153 A 20030106

OS MARPAT 140:27819

GI



I

AB The title compds. I [R1 represents (CO)h(NRa)j(CRb:CRc)kAr (wherein Ra,

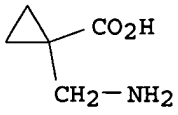
10760032-R3 AND R4 NON CICLYC

Rb, and Rc each independently represents hydrogen, halogeno, hydroxy, optionally substituted C1-6 alkyl, etc.); Ar = (un)substituted aromatic heterocyclic ring, etc.; h, j, k = 0 or 1; Cy is a 5- or 6-membered aromatic heterocycle; and V represents L-X-Y (wherein L is a single bond, optionally substituted C1-6 alkylene, etc.; X is a single bond, O, CO, etc.; and Y is hydrogen, halogeno, nitro, etc.); n = 0 - 4] are prepared Compds. of this invention in vitro showed IC50 values of 63 nM to 578 nM against JNK-3.

IT **139126-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazole derivs. as JNK inhibitors)

RN 139126-45-7 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



use older Reference leading Same compound!

RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:950974 CAPLUS

DN 140:16567

TI N-(Acylamino)benzene derivatives as selective monoamine oxidase B inhibitors

IN Jolidon, Synese; Rodriguez Sarmiento, Rosa Maria; Thomas, Andrew William; Wyler, Rene

PA F. Hoffmann-La Roche A.-G., Switz.

SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003099763	A1	20031204	WO 2003-EP5297	20030521
	WO 2003099763	C1	20040318		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003232883	A1	20031218	US 2003-445580	20030527
	US 6762320	B2	20040713		
	US 2004210079	A1	20041021	US 2004-839514	20040505
PRAI	EP 2002-11639	A	20020529		
	US 2003-445580	A1	20030527		

OS MARPAT 140:16567

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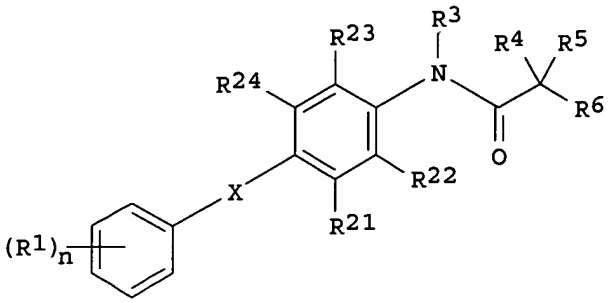
NRA

10760032-R3 AND R4 NON CICLYC



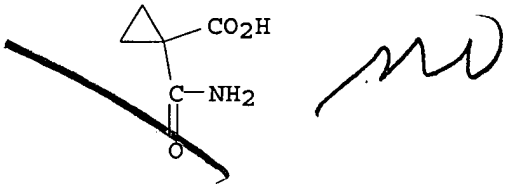
I

AB Title compds. such as I (R1 = halo, haloalkyl, cyano, alkoxy, haloalkoxy; n = 0, 1, 2, 3; X = CH2O, OCH2, CH2CH2, CH:CH, C.tplbond.C, etc.; R21, R22, R23, R24 = H, alkyl, halo, haloalkyl, OH, etc.; R3 = H, alkyl; R4, R5 = H, alkyl, alkoxy, alkoxycarbonyl, etc.; R6 = CONR7R8, alkoxycarbonyl, CN, etc.; R7, R8 = H, alkyl, NH2, OH) were prepared Thus, 4-(3-FC6H4CH2O)C6H4NHCOCH2CO2Me was prepared in 3 steps starting from 3-fluorobenzyl alc. and 1-fluoro-4-nitrobenzene. Several I were selective monoamine oxidase B inhibitors and are therefore useful in the treatment of diseases such as Alzheimer's disease and senile dementia.

IT **6914-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant with aniline derivative; acylanilides as monoamine oxidase B inhibitors)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:221465 CAPLUS

DN 138:255249

TI Preparation of piperazine and homopiperazine compounds useful in the treatment of thrombosis and to inhibit ADP-mediated platelet aggregation

IN Levy, Daniel E.; Smyth, Mark S.; Scarborough, Robert M.

PA Millennium Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 260 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003022214	A2	20030320	WO 2002-US28618	20020906
	WO 2003022214	A3	20040325		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,

10760032-R3 AND R4 NON CICLYC

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

	US 2003153556	A1	20030814	US 2002-237153	20020906
PRAI	US 2001-317192P	P	20010906		

OS MARPAT 138:255249

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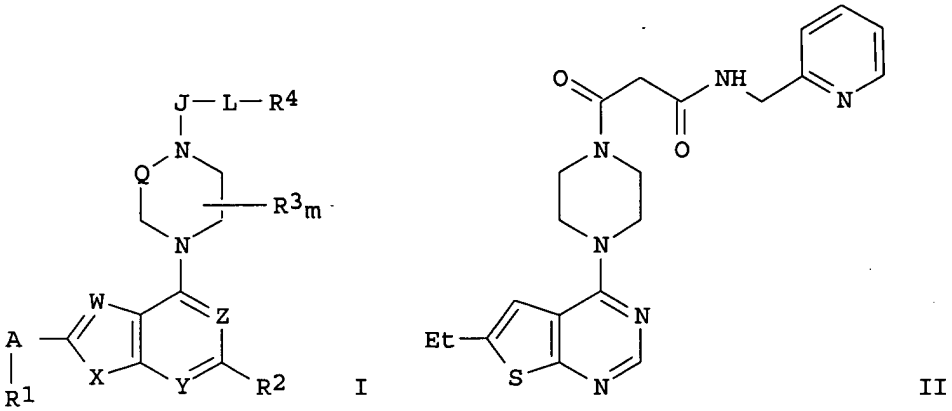
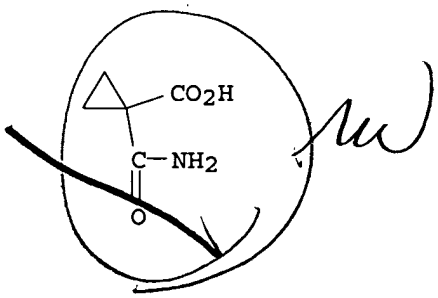


AB Piperazine and homopiperazine compds. I, wherein Q is (CH2)n; n is 1, 2; m is 0-4; W is N, CR5; X is S, O, NR6; Y is N, CR7; Z is N, CR8; J is CO, CS, CNR9, SO, SO2; A is O, S, NR10, CO, CH(OH); L is a direct link or a divalent linker; R1 is H, halo, CN, NO2, N3, alkyl, cycloalkyl, alkene, alkyne; R2 is H, halo, CN, NO2, N3, alkyl, cycloalkyl, alkene, alkyne, acyl; R3 is alkyl, cycloalkyl, acyl; R4 is H, F, CF3, CN, N3, NO2, alkyl, amino, alkylamino, cycloalkyl, heterocycloalkyl, heteroalkyl, fused bicycloalkyl, fused bicycloalkaryl, fused bicycloaryl; R5-R8 are independently H, alkyl, cycloalkyl; R9 is H, CN, NO2, alkyl; R10 is H, alkyl, acyl; are provided having a piperazine or homopiperazine ring which are useful in the treatment of thrombosis. Thus piperazine II was prepared and tested in vitro to inhibit ADP-mediated platelet aggregation (activity ranges are: > 20 μmol; 10-20 μmol; and < 10 μmol).

IT **6914-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperazine and homopiperazine compds. useful in treatment of thrombosis and to inhibit ADP-mediated platelet aggregation)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

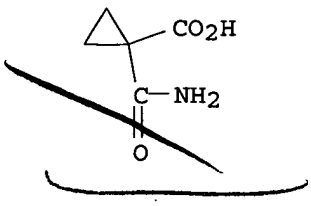
AN 2003:154399 CAPLUS

10760032-R3 AND R4 NON CICLYC

DN 138:204936
TI Preparation of heterocyclic compds. as integrase inhibiting antiviral agents
IN Kiyama, Ryuichi; Kanda, Yasuhiko; Tada, Yukio; Fujishita, Toshio; Kawasuji, Takashi; Takechi, Shozo; Fuji, Masahiro
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 663 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003016275	A1	20030227	WO 2002-JP8108	20020808
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1422218	A1	20040526	EP 2002-749384	20020808
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	BR 2002011750	A	20041013	BR 2002-11750	20020808
	US 2004229909	A1	20041118	US 2004-485394	20040130
PRAI	JP 2001-245071	A	20010810		
	JP 2001-370860	A	20011205		
	JP 2002-191483	A	20020628		
	WO 2002-JP8108	W	20020808		

OS MARPAT 138:204936
AB The title compds. RDC(:Z)C(Y):CRCRA [RC and RD in combination form a ring with the adjacent carbon atoms, provided that the ring may be a fused ring; Y represents hydroxy, mercapto, or amino; Z represents oxygen, sulfur, or NH; and RA represents N-containing aromatic heterocycle, etc.] are prepared Compds. of this invention in vitro showed IC50 values of 0.12 μg/mL to 2.9 μg/mL against integrase. Formulations are given.
IT **6914-74-5**, 1-(Aminocarbonyl)-1-cyclopropanecarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclic compds. as integrase inhibiting antiviral agents)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:696642 CAPLUS

10760032-R3 AND R4 NON CICLYC

DN 137:232915
TI Preparation of cryptophycin compounds as pharmaceuticals
IN Shih, Chuan
PA USA
SO U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S. Ser. No. 495,670.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002128185	A1	20020912	US 2001-990895	20011116
PRAI US 1998-29186	B2	19980225		
US 1998-29188	B2	19980225		
US 1998-29203	B2	19980225		
US 2000-495670	A2	20000201		

OS MARPAT 137:232915
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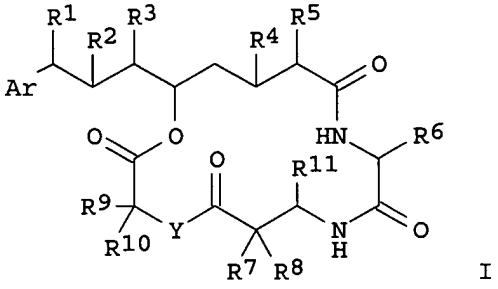
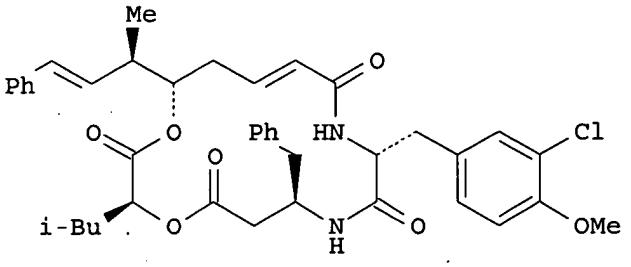


I



II

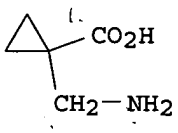
AB The invention provides novel cryptophycin compds. I [Ar = Ph which may be substituted by OH, alkoxy, halogen, or alkyl; R1 = halo and R2 = OH or R1R2 = O or a bond; R3 = alkyl; R4, R5 = H or together form a bond; R6 = benzyl, hydroxy-, alkoxy-, halohydroxy-, dihalohydroxy-, haloalkoxy-, or dihaloalkoxybenzyl; R7, R8 = H or together form a spiro group; R9 = H or alkyl; R10 = H; Y = O or NH] or pharmaceutically acceptable salts, which can can disrupt the microtubulin system of the cytoskeleton and are useful as antineoplastic or antifungal agents and for the treatment of cancer. The invention further provides a formulation for administering the novel cryptophycin compds. Thus, compound II was prepared via esterification, deprotection, and lactamization reactions. Compds. I were tested for cytotoxicity and antitumor activity.

IT **139126-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cryptophycin compds. as pharmaceuticals)

RN 139126-45-7 CAPLUS

10760032-R3 AND R4 NON CICLYC

CN Cyclopropanecarboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



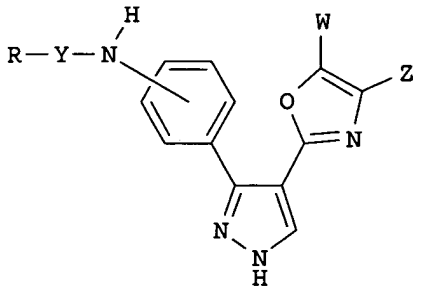
102

L3 ANSWER 11 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:615623 CAPLUS
DN 137:169517
TI Oxazolyl-pyrazole derivatives as protein kinase inhibitors, their preparation and combinatorial libraries, and their pharmaceutical use in the treatment of cancer and other diseases and disorders
IN Berta, Daniela; Felder, Eduard; Vulpetti, Anna; Villa, Marzia
PA Pharmacia Italia S.p.A., Italy
SO PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

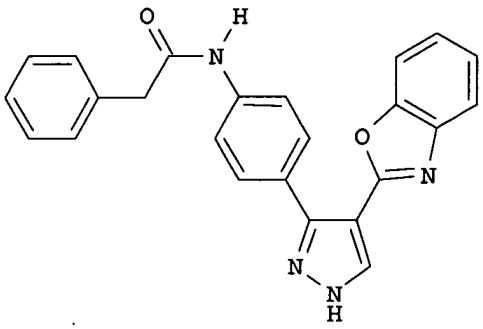
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002062804	A1	20020815	WO 2002-EP995	20020128
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2437260	AA	20020815	CA 2002-2437260	20020128
	EP 1377589	A1	20040107	EP 2002-714136	20020128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004520394	T2	20040708	JP 2002-563156	20020128
	US 2004180881	A1	20040916	US 2004-470859	20040415
PRAI	GB 2001-2687	A	20010202		
	WO 2002-EP995	W	20020128		

OS MARPAT 137:169517
GI

10760032-R3 AND R4 NON CICLYC



I

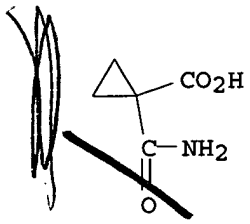


II

AB The method of treating protein kinase-linked diseases with oxazolyl-pyrazole derivs. I and their pharmaceutically acceptable salts is disclosed [wherein: R = H, alkyl, alkenyl, aryl, arylalkyl, (un)saturated cycloalkyl or cycloalkyloxy optionally condensed with 1 or 2 benzene rings, or optionally benzo-condensed 5- or 6-membered heterocyclyl or heterocyclylalkyl having 1 or 2 N/O/S atoms [all optionally substituted by one or more of: halo, NO2, cyano, OH, oxo, alkyl, alkoxyalkyl, perfluoroalkyl, (un)substituted aryl or 5- or 6-membered heterocyclyl having 1 or 2 N/O/S atoms, alkoxy, alkoxyalkyloxy, (un)substituted arylalkyloxy or aryloxy, alkylthio, alkylsulfonyl, arylthio, or arylsulfonyl, cycloalkyl, amino, alkylamino, dialkylamino, arylamino, alkylcarbonyl, alkyloxycarbonyl, alkylaminocarbonyl, aminocarbonyl, (un)substituted arylcarbonyl or heterocyclylcarbonyl, alkylcarbonylamino, alkyloxycarbonylamino, arylalkyloxycarbonylamino, arylcarbonylamino, aryloxycarbonylamino, carboxy, alkylcarbonyloxy, or arylcarbonyloxy]; Y = bond, CO, NHCO, SO2; WZ = benzo fusion, naphtho fusion, or an optionally benzocondensed 5- or 6-membered heterocycle having 1 or 2 N/O/S atoms, each optionally substituted by one or more of halo, nitro, cyano, alkyl, alkoxy, alkylsulfonyl, or aryl]. Also disclosed is a novel subset of I, including 382 individually named compds. I are useful in the treatment of diseases caused by and/or associated with an altered protein kinase activity, such as cancer, cell proliferative disorders, viral infections, autoimmune diseases and neurodegenerative disorders. Eleven examples are given, including solid-phase preparation of several compds. I and intermediates, and descriptions of 3 combinatorial libraries of 3874, 3172, and 2184 members, based on 4 claimed tables of reactants. For instance, Et 3-(3-nitrophenyl)pyrazole-4-carboxylate was bound to trityl chloride resin, saponified with NaOH in MeOH, and amidated with o-aminophenol. The resultant N-(2-hydroxyphenyl)amide was cyclized by Mitsunobu reaction to give a 1,3-benzoxazole derivative, followed by reduction of the nitro group to amino using SnCl2, amidation with PhCH2CO2H, and resin cleavage with TFA, to give title compound II. Inhibition assays against various kinases are described (no data).

IT **6914-74-5**, 1-(Aminocarbonyl)-1-cyclopropanecarboxylic acid
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial

study); RACT (Reactant or reagent)
(combinatorial reactant; preparation of oxazolylpyrazole derivs. as protein kinase inhibitors, and their combinatorial libraries and use as anticancer agents)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)

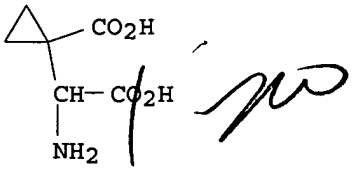


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:349172 CAPLUS
DN 136:355479
TI Reductive amination of alpha-keto-dicarboxylic acids
IN Rossen, Kai; Sarich, Martin; Latinovic, Milan; Rollmann, Claudia; Bommarius, Andreas
PA Degussa Aktiengesellschaft, Germany
SO Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 1203821	A2	20020508	EP 2001-125184	20011024
EP 1203821	A3	20040630		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
DE 10054492	A1	20020516	DE 2000-10054492	20001103
JP 2002199895	A2	20020716	JP 2001-334859	20011031
US 2002081671	A1	20020627	US 2001-985475	20011105
PRAI DE 2000-10054492	A	20001103		

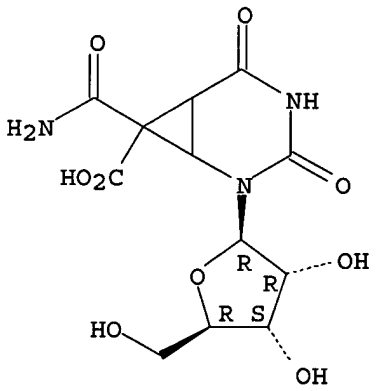
OS CASREACT 136:355479; MARPAT 136:355479
AB A process is provided for the reductive amination of a-keto-dicarboxylic acids by the enzymes amino acid dehydrogenase, leucine dehydrogenase or phenylalanine dehydrogenase. These enzymic reactions are coupled to the enzymic dehydrogenation of formate by formate dehydrogenase to regenerate the NADH required for the reductive amination.
IT **421548-64-3P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(reductive amination of alpha-keto-dicarboxylic acids)
RN 421548-64-3 CAPLUS
CN Cyclopropaneacetic acid, α-amino-1-carboxy- (9CI) (CA INDEX NAME)



10760032-R3 AND R4 NON CICLYC

L3 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:194991 CAPLUS
DN 136:355413
TI Synthesis of some antimicrobial pyrimidine nucleoside derivatives
AU El Bahnasawy, A. A.; Ahmed, A. F. Sayed; Koraiem, A. I. M.
CS Department of Chemistry, Faculty of Science, Zagazig University, Egypt
SO Aswan Science & Technology Bulletin (2001), 20, 46-60
CODEN: ASTBEQ; ISSN: 1110-0184
PB Aswan Faculty of Science
DT Journal
LA English
OS CASREACT 136:355413
AB Reactions of both of 6-chlorocytidine and 6-chlorouridine with ethylcyanoacetate were carried out under basic conditions to form cyclopropane derivs. Further alkaline reactions of these derivs. has been done. On the other hand, oxidation of hydroxamic acids in the presence of both of 5-bromo (hydroxy)-4-chloro(methoxy) pyrimidinone nucleoside afford cycloaddn. products. Reductive cleavage of the N-O bond of some produced cyclo adducts has been performed. The biol. activities of the prepared compds. towards gram-pos. and gram-neg. bacteria have been described.
IT **420805-09-0P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of antimicrobial pyrimidine nucleoside derivs. via cycloaddn and reductive bond cleavage)
RN 420805-09-0 CAPLUS
CN 2,4-Diazabicyclo[4.1.0]heptane-7-carboxylic acid, 7-(aminocarbonyl)-3,5-dioxo-2-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

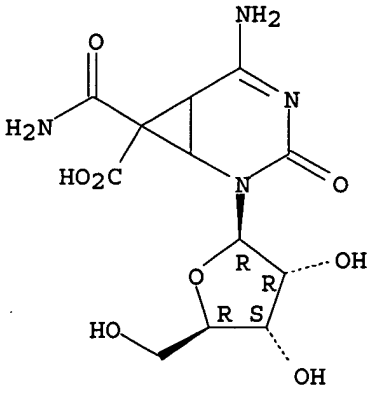
Absolute stereochemistry.



IT **420805-04-5P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of antimicrobial pyrimidine nucleoside derivs. via cycloaddn and reductive bond cleavage)
RN 420805-04-5 CAPLUS
CN 2,4-Diazabicyclo[4.1.0]hept-4-ene-7-carboxylic acid, 5-amino-7-(aminocarbonyl)-3-oxo-2-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

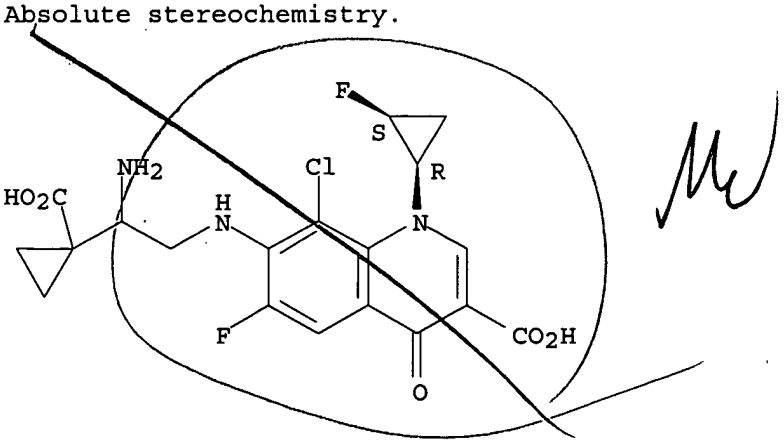
10760032-R3 AND R4 NON CICLYC



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:443690 CAPLUS
DN 136:241033
TI Structure study on sitafloxacin metabolites by LC/MS/MS
AU Xu, Xiaoping; Wang, Shu; He, Yingju; Chen, Cong; Nakaoa, Minoru
CS School of Pharmacy, West China University of Medical Sciences, Chengdu, 610041, Peop. Rep. China
SO Zhongguo Kangshengsu Zazhi (2001), 26(2), 108-111
CODEN: ZKZAEY; ISSN: 1001-8689
PB Zhongguo Kangshengsu Zazhishe
DT Journal
LA Chinese
AB Online identification of metabolites of sitafloxacin by LC/MS/MS was presented. The metabolites were confirmed by comparing with its authentic compds. by MS or MS/MS. The structures of metabolites D2-7 were identified as 7-R-8-chloro-1,4-dihydro-6-fluoro-1-(2-fluoro-1-cyclopropyl)-4-oxoquinoline-3-carboxylic acid (R = 7-oxo-5-azaspiro[2.4]hept-5-yl, 7-hydroxy-5-azaspiro[2.4]hept-5-yl, 7-acetamido-5- azaspiro[2.4]hept-5-yl, 2-acetamido-3-(1,2-ethylene)-4-hydroxybutylamino, or 3-carboxy-3-(1,2-ethylene)propylamino). The results showed that sitafloxacin was biotransformed with oxidation path way eliminated by liver microsomes.
IT **404566-29-6**
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(structure study on sitafloxacin metabolites by LC/MS/MS)
RN 404566-29-6 CAPLUS
CN 3-Quinolinecarboxylic acid, 7-[[2-amino-2-(1-carboxycyclopropyl)ethyl]amino]-8-chloro-6-fluoro-1-[(1R,2S)-2-fluorocyclopropyl]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

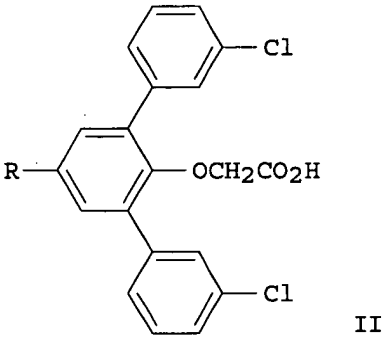


10760032-R3 AND R4 NON CICLYC

L3 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:255930 CAPLUS
DN 134:280608
TI Preparation of bi- and terphenylcarboxamides as protein tyrosine phosphatase inhibitors
IN Butera, John A.; Caufield, Craig E.; Graceffa, Russell F.; Greenfield, Alexander; Gundersen, Eric G.; Havran, Lisa Marie; Katz, Alan H.; Lennox, Joseph R.; Mayer, Scott C.; McDevitt, Robert E.
PA USA
SO U.S., 75 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6214877	B1	20010410	US 1999-307850	19990510
	US 2001018525	A1	20010830	US 2001-771469	20010126
	US 6451827	B2	20020917		
	US 2003083341	A1	20030501	US 2002-215438	20020809
	US 6765021	B2	20040720		
	US 2004214869	A1	20041028	US 2004-843026	20040511
PRAI	US 1998-108154P	P	19980512		
	US 1999-307850	A3	19990510		
	US 2001-771469	A3	20010126		
	US 2002-215438	A3	20020809		

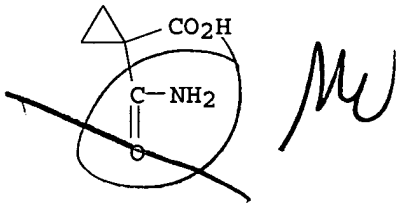
OS MARPAT 134:280608
GI



II

AB R1OZR [I; R = OH, alkyl, alkoxy, (hetero)aryl(alkyl), ureido, etc.; R1 = H, (carboxy)alkyl, etc.; Z = (un)substituted 2-aryl-1,4-phenylene] were prepared Thus, 4-(HO)C6H4CO2Et was brominated and the iodinated product etherified by HOCH2CH2OH to give Et 3-bromo-4-(2-hydroxyethoxy)-5-iodobenzoate which was arylated by 3-ClC6H4B(OH)2 and the product amidated by dodecylamine to give, after saponification, title compound II [R = Bu(CH2)8NHCO].
Data for biol. activity of I were given.
IT **6914-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bi- and terphenylcarboxamides as protein tyrosine phosphatase inhibitors)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)

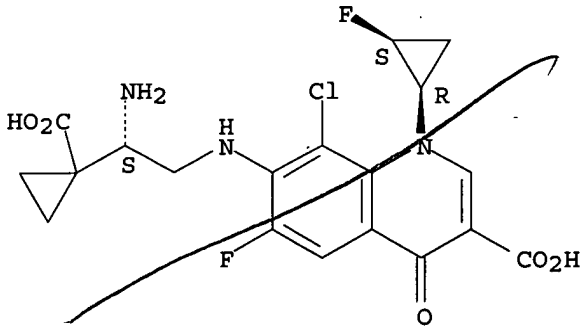
10760032-R3 AND R4 NON CICLYC



RE.CNT 112 THERE ARE 112 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:242125 CAPLUS
DN 135:70548
TI Simultaneous identification and separation of sitafloxacin metabolites by LC-MS
AU Xu, Xiao-ping; Wang, Shu; Chen, Cong; Nakaoka, Minoru
CS School of Pharmacy, West China University of Medical Sciences, Chengdu, 610041, Peop. Rep. China
SO Zhongguo Kangshengsu Zazhi (2000), 25(6), 424-427
CODEN: ZKZAEY; ISSN: 1001-8689
PB Zhongguo Kangshengsu Zazhishe
DT Journal
LA Chinese
AB Sitafloxacin metabolites were simultaneously separated and identified by LC-MS. After being administered with sitafloxacin, the urine and bile samples of rat, dog, monkey and human were determined resp. Nine metabolites (M1-M9) of sitafloxacin were identified. It is not only valuable for studying the metabolism of sitafloxacin but also provides structural candidate for developing new fluoroquinolones.
IT **347887-06-3**
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(simultaneous identification and separation of sitafloxacin metabolites by LC-MS)
RN 347887-06-3 CAPLUS
CN 3-Quinolinecarboxylic acid, 7-[[(2S)-2-amino-2-(1-carboxycyclopropyl)ethyl]amino]-8-chloro-6-fluoro-1-[(1R,2S)-2-fluorocyclopropyl]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:725485 CAPLUS
DN 133:296658

10760032-R3 AND R4 NON CICLYC

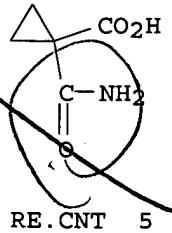
TI Preparation of desleucyl glycopeptide antibiotics
IN Kahne, Daniel; Walker, Suzanne; Silva, Domingos J.
PA The Trustees of Princeton University, USA; Incara Pharmaceuticals, Inc.
SO PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000059528	A1	20001012	WO 2000-US8559	20000331
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2370782	AA	20001012	CA 2000-2370782	20000331
	EP 1173193	A1	20020123	EP 2000-919942	20000331
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	US 6518243	B1	20030211	US 2000-540761	20000331
	US 2004110665	A1	20040610	US 2003-361603	20030211
PRAI	US 1999-127516P	P	19990402		
	US 2000-540761	A1	20000331		
	WO 2000-US8559	W	20000331		

AB Compds. that are analogs of glycopeptide antibiotics are disclosed. The compds. have the formula A1-A2-A3-A4-A5-A6-A7, where each of the groups A2 to A7 is a modified or unmodified α-amino acid residue, A1 is optional and, when present, is an organic group other than N-substituted leucine, and at least one of the groups A1 to A7 is linked via a glycosidic bond to one or more glycosidic groups each having one or more sugar residues, where at least one of said sugar residues is modified to bear at least one hydrophobic substituent. Methods of making these compds., compns. including these compds., and methods of using the compds. to treat infections in a host are also disclosed. Antibacterial test data are tabulated for > 350 compds. of the invention.

IT **6914-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of desleucyl glycopeptide antibiotics)

RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:764010 CAPLUS
DN 132:12200
TI Preparation of terphenyloxyalkanoic acids and analogs as protein-tyrosine

10760032-R3 AND R4 NON CICLYC

phosphatase inhibitors

IN Butera, John Anthony; Caufield, Craig Eugene; Graceffa, Russell Francis; Greenfield, Alexander; Gundersen, Eric Gould; Havran, Lisa Marie; Katz, Alan Howard; Lennox, Joseph Richard; Mayer, Scott Christian; McDevitt, Robert Emmett

PA American Home Products Corporation, USA

SO PCT Int. Appl., 277 pp.
CODEN: PIXXD2

DT Patent

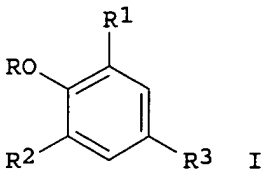
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9961410	A1	19991202	WO 1999-US10158	19990510
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2331056	AA	19991202	CA 1999-2331056	19990510
	AU 9940727	A1	19991213	AU 1999-40727	19990510
	EP 1077929	A1	20010228	EP 1999-924158	19990510
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	JP 2002516305	T2	20020604	JP 2000-550819	19990510
PRAI	US 1998-76709	A	19980512		
	WO 1999-US10158	W	19990510		

OS MARPAT 132:12200

GI



I

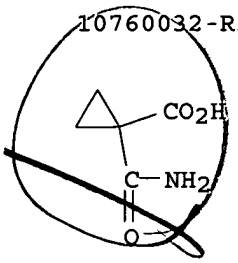
AB Title compds. [I; R = H, alkyl, SO2ZCO2H, CH2CO2H, (hetero)arylmethyl, etc.; R1,R2 = H, halo, alkyl, (hetero)aryl, etc.; R3 = alkyl, (hetero)aryl(alkyl), alkoxy(methyl), (un)substituted CONH2, etc.; Z = hydroxyphenyl] were prepared Thus, Et 2-bromo-4-(2-hydroxyethoxy)-5-iodobenzoate was condensed with 3-ClC6H4B(OH)2 and the product amidated by dodecylamine to give, after oxidation, I (R = CH2CO2H, R1 = R2 = C6H4Cl-3, R3 = dodecylcarbamoyl). Data for biol. activity of I were given.

IT **6914-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted biphenyl-, aryl, and terphenyloxyalkanoic acids as inhibitors for protein-tyrosine phosphatases in treatment of insulin resistance and hyperglycemia)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)

10760032-R3 AND R4 NON CICLYC



MW

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:165493 CAPLUS
DN 128:217640
TI Preparation of novel cryptophycins as microtubulin-disrupting antitumor and antifungal agents
IN Al-Awar, Rima S.; Ehlhardt, William J.; Gottumukkala, Subbaraju V.; Martinelli, Michael J.; Moher, Eric D.; Moore, Richard E.; Munroe, John E.; Norman, Bryan H.; Patel, Vinod F.; et al.
PA Eli Lilly and Company, USA; University of Hawaii; Wayne State University; Al-Awar, Rima S.; Ehlhardt, William J.; Gottumukkala, Subbaraju V.; Martinelli, Michael J.; Moher, Eric D.; Moore, Richard E.
SO PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9808506	A1	19980305	WO 1997-US15245	19970829
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	WO 9707798	A1	19970306	WO 1996-US13855	19960830
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI				
	CA 2263420	AA	19980305	CA 1997-2263420	19970829
	AU 9743300	A1	19980319	AU 1997-43300	19970829
	EP 957912	A1	19991124	EP 1997-941379	19970829
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 2001502297	T2	20010220	JP 1998-511080	19970829
PRAI	WO 1996-US13855	A	19960830		
	US 1997-38989P	P	19970226		
	US 1997-39529P	P	19970303		
	US 1995-2935P	P	19950830		
	WO 1997-US15245	W	19970829		

OS MARPAT 128:217640
GI

102(b) 9/97 claim 1 and 3 5

10760032-R3 AND R4 NON CICLYC

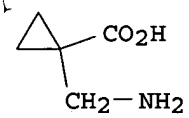
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB This invention provides novel cryptophycin compds. I [G = C1-12 alkyl, C2-12 alkenyl, (un)substituted aryl or heteroaryl; R1 = halo, SR, OR, NH2, mono- or di-C1-6 alkylamino, tri-C1-6 alkylammonium, C1-6 alkylthio, di-C1-6 alkylsulfonium, C1-6 alkylsulfonyl, C1-6 alkylphosphonyl, R2 = OH, NH2, NR, SH; R1R2 = form double bond, 3-membered ring; R = H, C1-6 alkyl; R3 = lower alkyl; R4, R5 = H, double bond; R6 = (un)substituted C1-6 alkyl, C3-8 cycloalkyl, heteroaryl, aryl, alkylaryl; R7 = H, lower alkyl, C1-3 alkyl-NR51R52, OR51; R8 = H, lower alkyl; or R7R8 form cyclopropyl ring; R51, R52 = independently C1-3 alkyl; R9 = H, lower alkyl, unsatd. lower alkyl, lower alkyl-C3-5 cycloalkyl; R10 = H, lower alkyl; or R9R10 form cyclopropyl ring; R11 = H, OH, alkyl, Ph, substituted Ph, CH2Ph, substituted CH2Ph; R14 = H, lower alkyl; R30 = H, C1-6 alkyl; X = O, NH, alkylamino; Y = O, NH, alkylamino; with provisos] and pharmaceutically acceptable salts thereof, useful for disrupting the microtubulin system, as antineoplastic agents, antifungal agents, and for the treatment of cancer. The invention further provides a formulation for administering the novel cryptophycin compds. Thus, coupling of cyclopropanecarboxylic acid II (Boc = CO2CMe3) (preparation given) with cryptophycin fragment III, followed by deprotection, cyclization, and chlorohydrin formation gave novel cryptophycin IV. Compds. of this invention are useful against pathogenic fungi and were evaluated against a broad spectrum of murine and human tumors implanted in mice, including drug-resistant tumors.

IT **139126-45-7P**, LY 257141
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel cryptophycins as microtubulin-disrupting antitumor and antifungal agents)

RN 139126-45-7 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



Same Compound !

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:151085 CAPLUS

DN 128:256692

TI The cycloalkane derivatives and carboxylic acid derivatives for preservation of cut flower

IN Sugiyama, Nagyoshi; Oritani, Takayuki

PA Otsuka Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 10059801	A2	19980303	JP 1997-163402	19970604
PRAI JP 1996-166706	A	19960605		

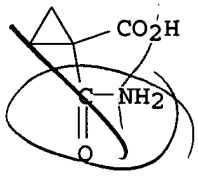
AB Freshness of cut flower is preserved with cycloalkane derivs. and/or carboxylic acid derivs. The method is low in cost, free of environmental pollution, and highly effective.

IT **6914-74-5 139126-45-7**

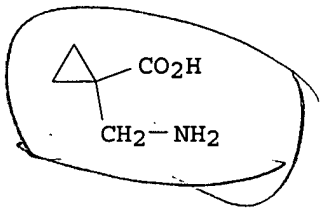
10/26(b)

10760032-R3 AND R4 NON CICLYC

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(cycloalkane derivs. and carboxylic acid derivs. for preservation of cut flower)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)

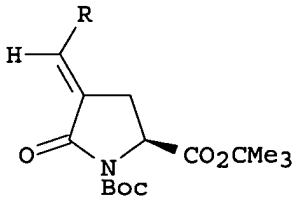


RN 139126-45-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:764140 CAPLUS
DN 128:102358
TI Stereospecific synthesis of naturally-occurring 4-alkylideneglutamic acids, 4-alkylglutamates and 4-alkylprolines 1
AU Moody, Claire M.; Young, Douglas W.
CS CPES, Sussex Centre for Biomolecular Design and Drug Development, University of Sussex, Falmer, Brighton, BN1 9QJ, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (23), 3519-3530
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 128:102358
GI

10760032-R3 AND R4 NON CICLYC



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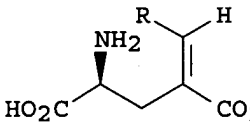

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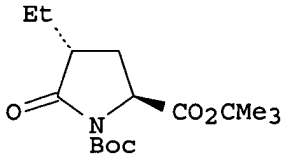
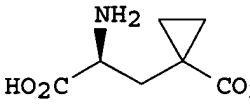
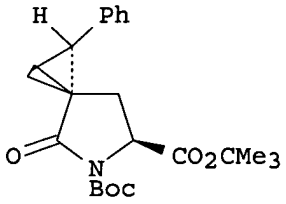


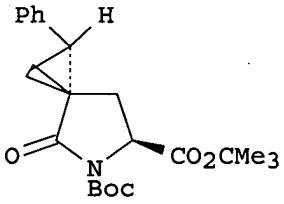
III



IV



V



VI

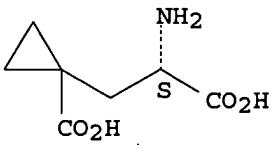
AB The enaminone I (R = NMe2), prepared from L-pyroglutamic acid, reacts with DIBAL and Grignard reagents in an apparent 1,4-manner to afford a variety of alkylidene derivs. I (R = H, Me, Et, Ph, C.tplbond.CH, CH:CH2) which, except for the vinyl derivs. , are formed only as the E-isomers. Three of these have been converted to the 4-alkylideneglutamic acids II (R = H, Me, Et), which are identical to known natural products, the synthesis confirming II (R = Me, Et) as the E-isomers. Catalytic reduction of the 4-alkylidenepyroglutamate derivs. I is stereospecific and affords an effective route to (2S,4S)-4-alkylglutamic acids and (2S,4S)-4-alkylprolines. Cuprate addition to the enone I (R = H) affords access to the (2S,4R)-epimer III and carbene addition allows cyclopropylglutamic acids IV-VI to be prepared

IT **158196-44-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereospecific synthesis of naturally-occurring 4-alkylideneglutamic acids, 4-alkylglutamates and 4-alkylprolines)

RN 158196-44-2 CAPLUS

CN Cyclopropanepropanoic acid, α-amino-1-carboxy-, hydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



● HCl

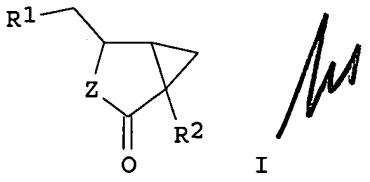
RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10760032-R3 AND R4 NON CICLYC

L3 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:502305 CAPLUS
DN 127:135716
TI Preparation of 2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxamides and -amines as synthetic intermediates
IN Kleemis, Wolfgang
PA Huels AG, Germany; Degussa AG
SO Ger. Offen., 13 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 19600034	A1	19970703	DE 1996-19600034	19960102
DE 19600034	C2	20031224		
PRAI DE 1996-19600034		19960102		

OS MARPAT 127:135716
GI



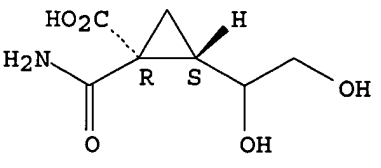
I

AB Title compds. [I; R1 = OH or acyloxy; R2 = CONH2 or (un)substituted NH2; Z = O, S, (un)substituted imino] were prepared Thus, cis-Me 1-carbamoyl-2-vinylcyclopropanecarboxylate was treated with H2O2 and the resulting glycol heated to give 92.5% I (R1 = OH, R2 = CONH2, Z = O) in a 75:25 diastereomeric ratio.

IT **192947-89-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-oxo-3-oxabicyclo[3.1.0]hexane-1-carboxamides and -amines as synthetic intermediates)

RN 192947-89-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(1,2-dihydroxyethyl)-, (1α,2α)-[partial]- (9CI) (CA INDEX NAME)

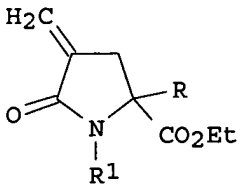
Relative stereochemistry.



L3 ANSWER 23 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:130876 CAPLUS
DN 126:238627
TI Synthesis of 2-substituted 4-methyleneglutamic acids and their cyclopropyl analogs
AU Guillena, Gabriela; Mico, Irene; Najera, Carmen; Ezquerra, Jesus; Pedregal, Concepcion

10760032-R3 AND R4 NON CICLYC

CS Fac. Ciencias, Univ. Alicante, Alicante, 03080, Spain
SO Anales de Quimica International Edition (1996), 92(6), 362-369
CODEN: AQIEFZ
PB Springer
DT Journal
LA English
OS CASREACT 126:238627
GI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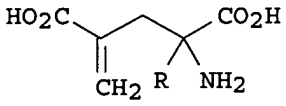
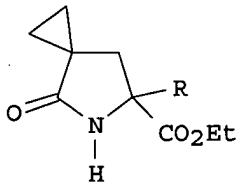
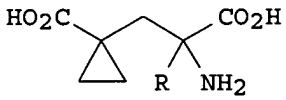

II

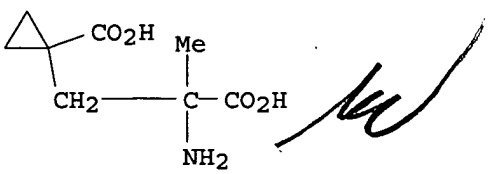

III


IV

AB The alkylation of the dianion derived from 4-methylenepyroglutamate I (R = R1 = H) allows the synthesis of 2-substituted 4-methyleneglutamates I (R = Me, CH2CH:CH2, CH2CHMe2, CH2Ph, CH2CH2Ph; R1 = Boc), after final N-Boc protection. Substituted I can also be prepared by alkylation at the 2-position of the dianion derived from Et pyroglutamate, followed by methylenation at the 4-position and final N-Boc protection. Hydrolysis of substituted methylene derivs. I led to the preparation of 2-substituted 4-methyleneglutamic acids II. The cyclopropanation of 2-alkylated-4-methylenepyroglutamates I (R1 = H) with diazomethane catalyzed by Pd(OAc)2 affords the cyclopropyl analogs III, which are converted into the corresponding 2-substituted 4,4-ethyleneglutamic acids IV.

IT **188548-29-0P 188548-30-3P 188548-31-4P**
188548-32-5P 188548-33-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted methyleneglutamic acids and their cyclopropyl analogs)

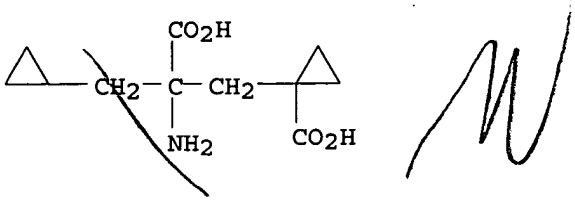
RN 188548-29-0 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-α-methyl- (9CI) (CA INDEX NAME)



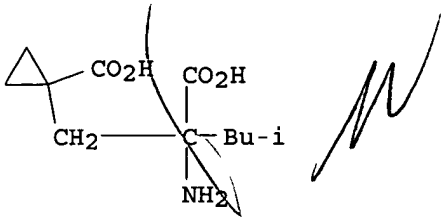
RN 188548-30-3 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-α-

10760032-R3 AND R4 NON CICLYC

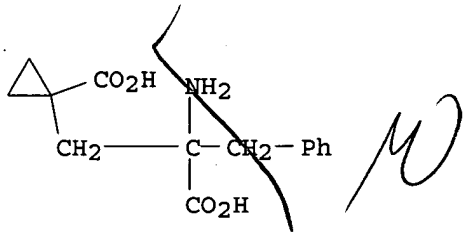
(cyclopropylmethyl)- (9CI) (CA INDEX NAME)



RN 188548-31-4 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-α-(2-methylpropyl)- (9CI) (CA INDEX NAME)

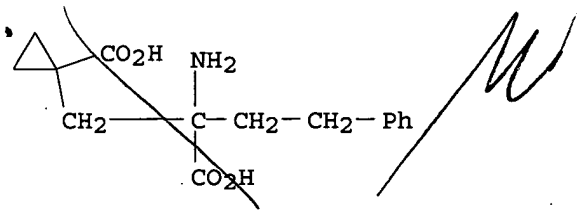


RN 188548-32-5 CAPLUS
CN Phenylalanine, α-[(1-carboxycyclopropyl)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 188548-33-6 CAPLUS
CN Benzenebutanoic acid, α-amino-α-[(1-carboxycyclopropyl)methyl]- (9CI) (CA INDEX NAME)

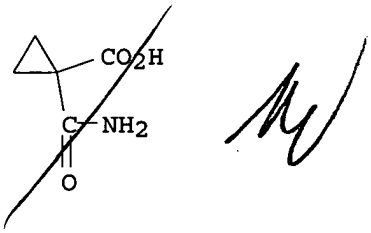


RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:380900 CAPLUS
DN 125:59041
TI Synthesis of 1-aminocyclopropane-1-carboxylic acid
AU Il'yasov, E. A.; Galust'yan, G. G.
CS Inst. Khim. Rastit. Veshchestv, AN RUz, Tashkent, Uzbekistan

10760032-R3 AND R4 NON CICLYC

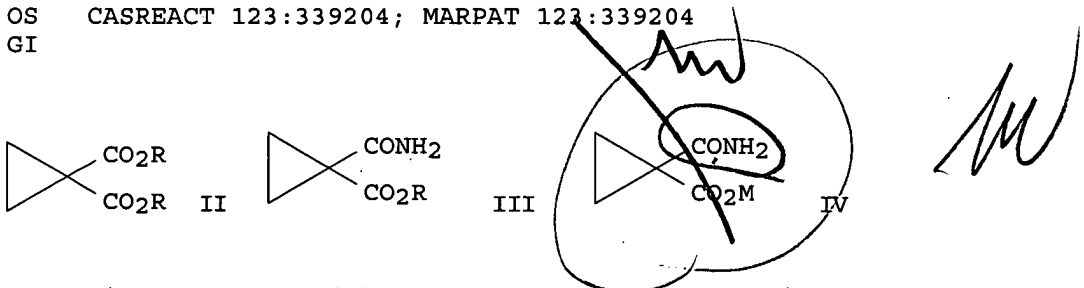
SO Khimiya Prirodnykh Soedinenii (1995), (6), 855-857
CODEN: KPSUAR; ISSN: 0023-1150
PB Fan
DT Journal
LA Russian
AB 1-Amino-1-cyclopropanecarboxlic acid was prepared by alkylation of Et cyanoacetate with 1,2-dibromoethane, followed treatment solns. containing NaOH, H2O2, and Br2-NaOH.
IT **6914-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of aminocyclopropanecarboxylic acid)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:954752 CAPLUS
DN 123:339204
TI Preparation of 1-aminocyclopropane carboxylic acid hydrochloride.
IN Kleemiss, Wolfgang; Feld, Marcel
PA Huels A.-G., Germany
SO Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 676390	A1	19951011	EP 1995-101384	19950202
	EP 676390	B1	19970102		
	R: CH, DE, ES, FR, GB, IT, LI				
	DE 4411777	A1	19951012	DE 1994-4411777	19940406
	JP 07278077	A2	19951024	JP 1995-79191	19950404
	US 5569781	A	19961029	US 1995-416989	19950405
PRAI	DE 1994-4411777	A	19940406		

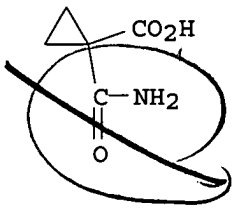
OS CASREACT 123:339204; MARPAT 123:339204
GI



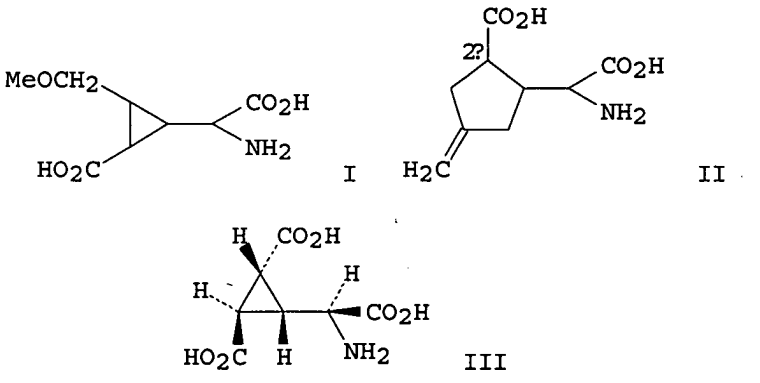
AB Title compound (I) was prepared from diesters (II; R = C1-8 alkyl) via ester-amides (III) and amide-salts (IV; M = alkali- or alkaline earth metal). Thus, II (R = Me) in MeOH was treated 10 h with NH3 at 20° to give 92.5% III (R = Me). This was heated with aqueous NaOH at 40° for 20 min. and the resulting homogeneous solution was added with aqueous NaOCl over 1 h
to a mixing vessel and conducted through a tube reactor at 80° followed by acidification with HCl to give 80% I.

10760032-R3 AND R4 NON CICLYC

IT **6914-74-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-aminocyclopropane carboxylic acid hydrochloride from 1,1-cyclopropanedicarboxylate diesters)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:15890 CAPLUS
DN 122:81918
TI Syntheses of conformationally constrained glutamate analogs
AU Shimamoto, K.; Raghavan, S.; Ouerfelli, O.; Ohfune, Y.
CS Suntory Inst. Bioorg. Res., Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1993), 35th, 559-66
CODEN: TYKYDS
DT Journal
LA Japanese
GI



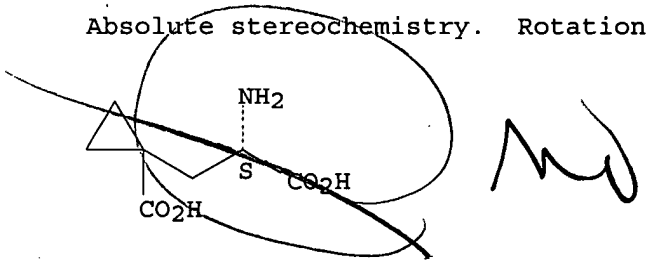
I II III

AB Six diastereomers of 2-(2-carboxy-3-methoxymethylcyclopropyl)glycine I, 3 diastereomers of 2-(2-carboxy-4-methylenecyclopentyl)glycine II, 3 analogs of 4-substituted glutamic acids, and 2-(2,3-dicarboxycyclopropyl)glycine III were prepared to examine the conformational requirements of Glu receptors as well as to develop new Glu agonists. The syntheses of I were characterized by (1) intramol. cyclopropanation of diazoacetamides with (E)- or (Z)-allyl ethers and (2) inversion of cis-substituted α-cyclopropyl acyl anion to the trans ester. Palladium catalyzed [3+2] cycloaddn. of (E)- or (Z)-α,β-unsatd. trifluoroethyl esters with a trimethylenemethane equivalent furnished the desired cycloadducts which were converted to the 2'R isomers II. (2'S)-II was prepared by the stereoselective 1,4-addition of a trimethylenemethane species to a (Z)-ester. Aminocarbonylation of the propargylglycine derivative prepared

from L-aspartic acid gave the 4-methyleneglutamic acid derivative which was used for the syntheses of 4-substituted glutamic acids. The synthesis of III was carried out starting from a common trans ester synthetic intermediate of I. Cis-cyclopropyl-substituted I (cis-I), which freeze the rotation of the α-amino acid moiety, showed similar activities to their parent (carboxycyclopropyl)glycines, suggesting the conformation of α-amino acid moiety of Glu for activating metabotropic receptors and N-methyl-D-asparate (NMDA) receptors. Trans-I and II were classified as kainate (KA) receptor agonists. Their conformational relationship suggests that the folded form of Glu is also responsible for activating KA receptors. Moreover, III was a potent and selective metabotropic receptor agonist.

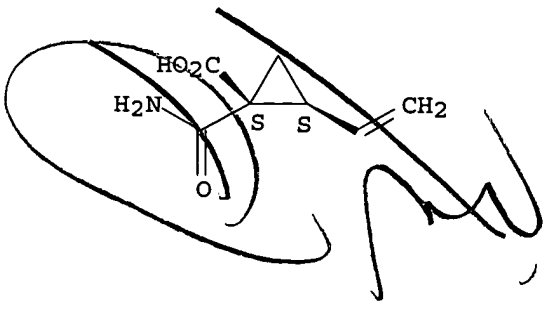
IT **151139-87-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(glutamate receptor agonist activity of)
RN 151139-87-6 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



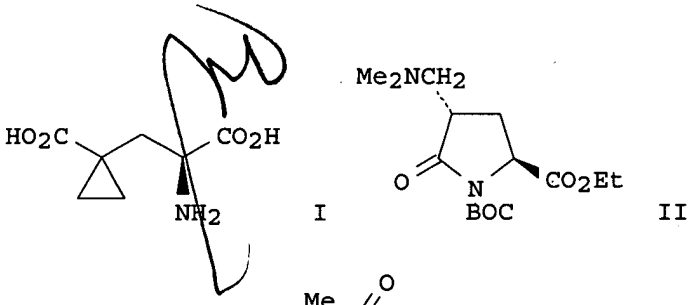
L3 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:655267 CAPLUS
DN 121:255267
TI A convenient synthesis of methyl (Z)-1-carbamoyl-2-ethenylcyclopropanecarboxylate and (Z)-1-carbamoyl-2-ethenylcyclopropanecarboxylic acid
AU Galgoci, Michelle; Davidson, Janel E.; Harrington, Clinton K.; Hasha, Dennis L.; Goralski, Christian T.
CS Dow Chemical Co., Midland, MI, 48674, USA
SO Synthetic Communications (1994), 24(17), 2477-83
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
OS CASREACT 121:255267
AB A simple method for the preparation of the title compds. via the reaction of di-Me 2-ethenylcyclopropane-1,1-dicarboxylate with 6M ammonia in methanol is described.
IT **158665-23-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 158665-23-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-ethenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



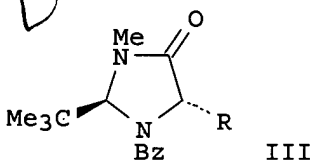
10760032-R3 AND R4 NON CICLYC

L3 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:631298 CAPLUS
DN 121:231298
TI Efficient synthesis of 4-methylene-L-glutamic acid and its cyclopropyl analog
AU Ezquerra, Jesus; Pedregal, Concepcion; Mico, Irene; Najera, Carmen
CS Cent. Invest. Lilly S. A., Valdeolmos, 28130, Spain
SO Tetrahedron: Asymmetry (1994), 5(5), 921-6
CODEN: TASYE3; ISSN: 0957-4166
DT Journal
LA English
OS CASREACT 121:231298
GI



I

II



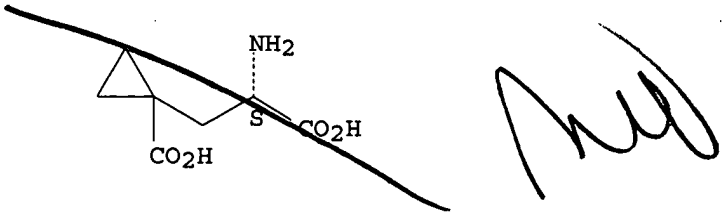
III

AB Title compds. L-NHCH(CO2H)CH2C(CO2H):CH2 and cyclopropyl analog I were obtained from protected pyroglutamate Boc-pGlu-OEt (Boc = Me3CO2C) in 2 and 3 steps, resp. Key methylenepyroglutamate intermediate II was prepared by reaction of the protected pyroglutamate lithium lactam enolate with Eschenmoser's salt. Cyclopropyl derivative I was also prepared from imidazolidone III (R = H) in 3 steps. The intermediate III [R = CH2C(CO2Bu):CH2] was obtained by diastereoselective reaction of the lithium enolate of III (R = H) with Bu (2-tosylmethyl)acrylate.

IT **158196-44-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 158196-44-2 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-, hydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

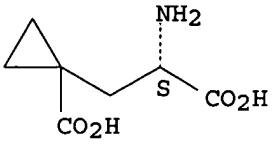


● HCl

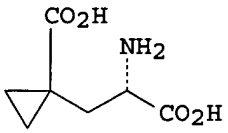
10760032-R3 AND R4 NON CICLYC

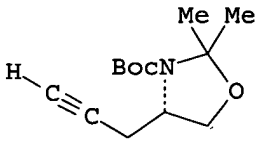
IT **151139-87-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from pyroglutamic acid)
RN 151139-87-6 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



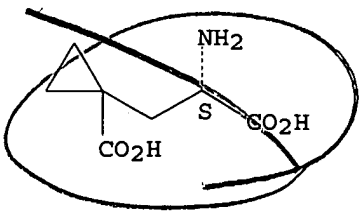
L3 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:650414 CAPLUS
DN 119:250414
TI Efficient synthesis of 4-methylene-L-glutamic acid and its analogs
AU Ouerfelli, Ouathek; Ishida, Michiko; Shinozaki, Haruhiko; Nakanishi, Koji; Ohfune, Yasufumi
CS Suntory Inst. Bioorg. Res., Osaka, 618, Japan
SO Synlett (1993), (6), 409-10
CODEN: SYNLES; ISSN: 0936-5214
DT Journal
LA English
OS CASREACT 119:250414
GI


I


II

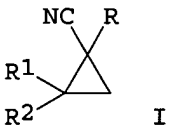
AB Three analogs of 4,4-disubstituted L-glutamate, (S)-H2C:C(CO2C)CH2CH(NH2)CO2H, (S)-HO2CCMe2CH2CH(NH2)CO2H, and cyclopropane I, were prepared via a regioselective aminocarbonylation of optically active propargylglycine equivalent II prepared from Boc-L-Asp(OCH2Ph)-OH (Boc = Me3CO2C).
IT **151139-87-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, via regioselective aminocarbonylation of propargylglycine synthon)
RN 151139-87-6 CAPLUS
CN Cyclopropanepropanoic acid, α-amino-1-carboxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



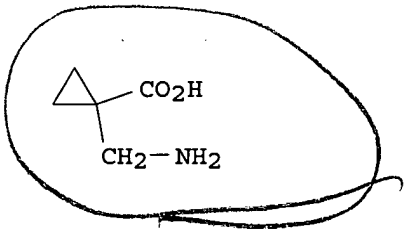
10760032-R3 AND R4 NON CICLYC

L3 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:105655 CAPLUS
DN 116:105655
TI Novel synthesis of 1-cyanocyclopropanecarboxylic acid and its application to the synthesis of amino acids containing cyclopropane rings
AU Ohno, Mitsuru; Tanaka, Haruhisa; Komatsu, Mitsuo; Ohshiro, Yoshiki
CS Fac. Eng., Osaka Univ., Suita, 565, Japan
SO Synlett (1991), (12), 919-20
CODEN: SYNLES; ISSN: 0936-5214
DT Journal
LA English
OS CASREACT 116:105655
GI



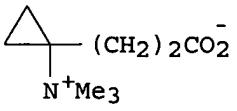
I

AB 1-Cyano-1-trimethylsilylcyclopropanes I (R = SiMe3, R1 = R2 = H, Ph; R1 = Ph, R2 = H) were efficiently converted to 1-cyanocyclopropane-1-carboxylic acids I (R = CO2H, R1, R2 = same) in the presence of a fluoride ion source (CsF) under CO2 atmosphere. This transformation provides a novel route to 1-aminocyclopropane-1-carboxylic acid, which is found in many plants, and to its homolog (1-aminomethylcyclopropane-1-carboxylic acid).
IT **139126-45-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 139126-45-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)

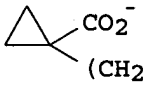


L3 ANSWER 31 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:212931 CAPLUS
DN 112:212931
TI Inhibition of γ-butyrobetaine hydroxylase by cyclopropyl-substituted γ-butyrobetaines
AU Petter, Russell C.; Banerjee, Satyajit; Englard, Sasha
CS Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SO Journal of Organic Chemistry (1990), 55(10), 3088-97
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 112:212931
GI

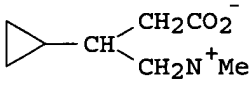
10760032-R3 AND R4 NON CICLYC



I



II



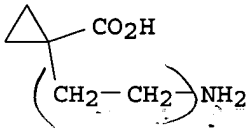
III

AB γ-Butyrobetaine hydroxylase EC 1.14.11.1) of Pseudomonas sp. AK1 catalyzes the final step in the biosynthesis of carnitine. A stepwise, homolytic mechanism has previously been proposed. Cyclopropyl-substituted substrate analogs, I, II, and III, were synthesized and evaluated as inhibitors of the enzyme with a view toward their potential as free radical clock probes for radical transients. Betaines I and III were competitive inhibitors and provided Ki values of 12.9 and 7.9 mM, resp. Betaine II was a noncompetitive inhibitor with Kii of 1.54 mM and for Kis of 1.96 mM. In each case, enzyme activity was determined by measurement of (a) the 14CO2 liberated from the coupled decarboxylation of [1-14C]-2-oxoglutarate and (b) the 3H released into the aqueous medium from [2,3-3H]-γ-butyrobetaine added as substrate. None of the 3 cyclopropyl derivs. exhibited turnover, and preincubation of these substrate analogs with γ-butyrobetaine hydroxylase did not result in a time-dependent loss of activity greater than that of the controls. The results were discussed in terms of the conformations of the inhibitors relative to those of the substrate.

IT **126822-37-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)

RN 126822-37-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(2-aminoethyl)- (9CI) (CA INDEX NAME)



(103) analog

L3 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:134732 CAPLUS

DN 110:134732

TI Synthesis of 1-aminocyclopropane-1-carboxylic acid by phase transfer method

AU Guo, Shuhao; Du, Ruli

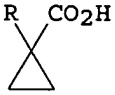
CS Dep. Chem., Jinan Univ., Guangzhou, Peop. Rep. China

SO Jinan Liyi Xuebao (1988), (1), 106-8
CODEN: JLXUDG; ISSN: 0255-8289

DT Journal

LA Chinese

GI



I

an extra CH_2

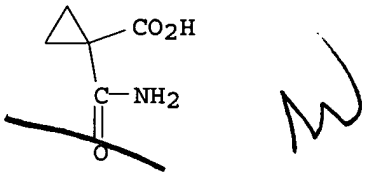
10760032-R3 AND R4 NON CICLYC

AB Phase-transfer reaction of NCCH2CO2Et with BrCH2CH2Br gave 86.5% cyclopropane I (R = cyano), hydrolysis of which gave 84.0% amide I (R = CONH2). Phase-transfer Hofmann reaction of the latter compound gave 80.3% the title compound (I, R = NH2).

IT **6914-74-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Hofmann reaction of)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 33 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:528440 CAPLUS

DN 109:128440

TI Preparation of 1-aminocyclopropane-1-carboxylic acid

IN Davidovich, Yu. A.; Shtil'man, M. I.; Kornakov, M. Ya.

PA Institute of Heteroorganic Compounds, Academy of Sciences, USSR, USSR

SO U.S.S.R.
From: Otkrytiya, Izobret. 1987, (20), 102.
CODEN: URXXAF

DT Patent

LA Russian

FAN.CNT 1

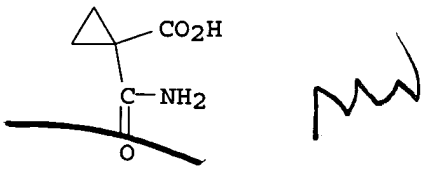
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI SU 1313851	A1	19870530	SU 1985-3886907	19850418
PRAI SU 1985-3886907		19850418		

AB Reaction of di-Et malonate and BrCH2CH2Br in the presence of K2CO3 gives di-Et cyclopropane-1,1-dicarboxylate. This is then hydrolyzed and converted to the monoamide which undergoes Hofmann reaction to give the title compound

IT **6914-74-5P**, Cyclopropane-1,1-dicarboxylic acid monoamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Hofmann reaction of)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



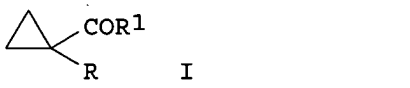
L3 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:614881 CAPLUS

DN 103:214881

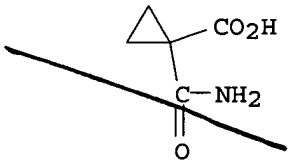
10760032-R3 AND R4 NON CICLYC

TI Synthesis of 1-aminocyclopropane-1-carboxylic acid - a new type of plant growth regulator
AU Zhu, Xuxiang; Guo, Qizhen
CS Dep. Chem., Xiamen Univ., Xiamen, Peop. Rep. China
SO Youji Huaxue (1985), (2), 153-5
CODEN: YCHHDX; ISSN: 0253-2786
DT Journal
LA Chinese
OS CASREACT 103:214881
GI



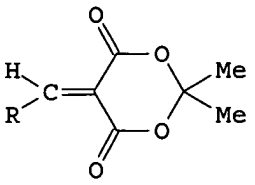
I

AB The title compound (I; R = NH2, R1 = OH) was prepared either by cyclocondensation of MeCOCH2CO2Et with BrCH2CH2Br, then aminolysis of I (R = CO2Et, R1 = Me), followed by Hofmann and haloform reactions of I (R = CONH2, R1 = Me) in 10% total yield; or by cyclocondenstion of NCCH2CO2Et with BrCH2CH2Br, then hydrolysis of I (R = cyano, R1 = OEt), followed by Hofmann reaction of I (R = CONH2, R1 = OH) in 45% total yield. The latter method is applicable for industrial manufacture of the title compound
IT **6914-74-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Hofmann reaction of)
RN 6914-74-5 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)

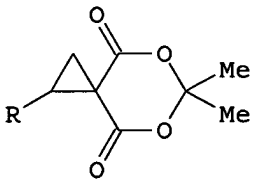


L3 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1985:453711 CAPLUS
DN 103:53711
TI Synthesis of E- and Z-1-amino-2-aryl(alkyl)cyclopropanecarboxylic acids via meldrum derivatives
AU Izquierdo, M. L.; Arenal, I.; Bernabe, M.; Fernandez Alvarez, E.
CS Inst. Quim. Org. Gen., CSIC, Madrid, 6, Spain
SO Tetrahedron (1985), 41(1), 215-20
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 103:53711
GI

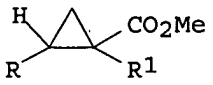
10760032-R3 AND R4 NON CICLYC



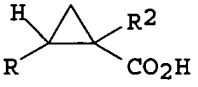
I



II



III



V

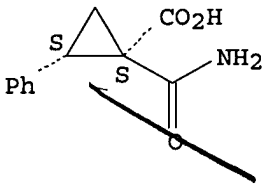
AB Meldrum acid derivs. I (R = Ph, 3-ClC6H4, 4-FC6H4, 4-MeOC6H4, etc.) were treated with CH2SOMe2 to give dioxaspiro[2,5]octanes II, which were treated with NaOMe or NH4OH to give cyclopropanes III (R1 = CO2H) (IV) and V (R2 = CONH2) (VI), resp. IV underwent Curtius-type reactions to give III (R1 = NCO) (VII), whereas VI were treated with hypobromite to give V CR2 = NHAc) (VIII). VII and VIII were hydrolyzed to give the corresponding 1-amino-1-cyclopropanecarboxylic acid derivative

IT **97364-47-1P 97364-48-2P 97364-49-3P**
97364-50-6P 97364-51-7P 97364-52-8P
97364-53-9P 97364-54-0P 97364-55-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 97364-47-1 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-phenyl-, cis- (9CI) (CA INDEX NAME)

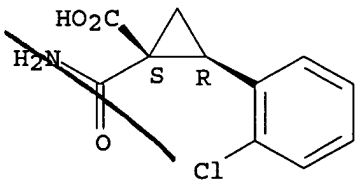
Relative stereochemistry.



RN 97364-48-2 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(2-chlorophenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

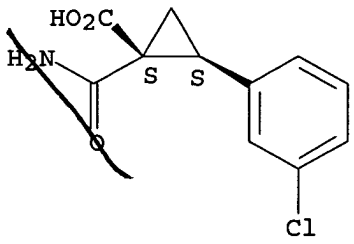


RN 97364-49-3 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(3-chlorophenyl)-, cis- (9CI) (CA INDEX NAME)

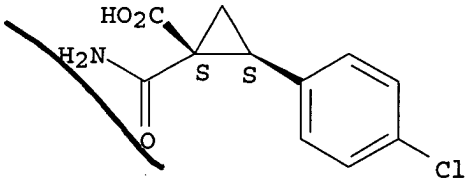
Relative stereochemistry.

10760032-R3 AND R4 NON CICLYC



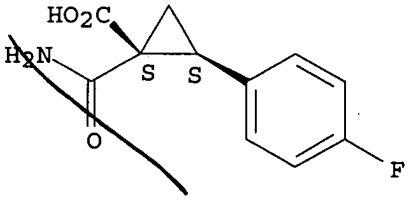
RN 97364-50-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(4-chlorophenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



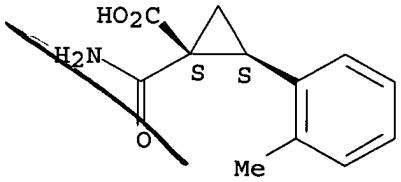
RN 97364-51-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(4-fluorophenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 97364-52-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(2-methylphenyl)-, cis- (9CI) (CA INDEX NAME)

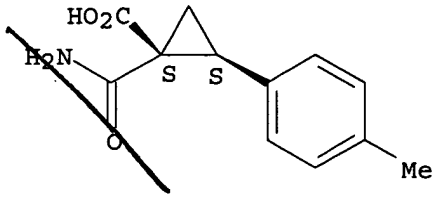
Relative stereochemistry.



RN 97364-53-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(4-methylphenyl)-, cis- (9CI) (CA INDEX NAME)

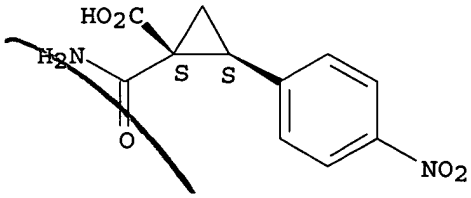
Relative stereochemistry.

10760032-R3 AND R4 NON CICLYC



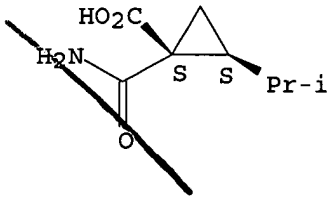
RN 97364-54-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(4-nitrophenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 97364-55-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)-2-(1-methylethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



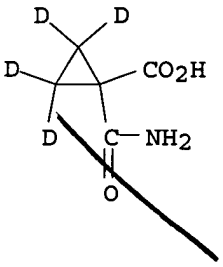
L3 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1984:506417 CAPLUS
DN 101:106417
TI Stereochemical studies on the reactions catalyzed by the PLP-dependent enzyme 1-aminocyclopropane-1-carboxylate deaminase
AU Liu, Hungwen; Auchus, Richard; Walsh, Christopher T.
CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SO Journal of the American Chemical Society (1984), 106(18), 5335-48
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CASREACT 101:106417
AB The stereochem. course of 1-aminocyclopropane-1-carboxylate (ACPC) deaminase, which catalyzes the fragmentation of the cyclopropane substrate to α-ketobutyrate and NH3, was studied by using substrates stereospecifically labeled with deuterium and(or) tritium; important information about the process occurring at the active site during enzymic conversion was thus obtained. These results can be summarized as follows: (1) ring cleavage is regiospecific and only occurs between the pro-S and the α-C atom of ACPC; (2) β-H abstraction is pro-R stereospecific and the reprotonation at the β-C atom is mediated by the same enzyme base which is partially shielded and located at the si face relative to the α-C atom; (3) the preferred conformation of the

β,γ-olefinic pyridoxal 5'-phosphate-p-quinoid α-anion complex is cisoid, and the geometry of the terminal double bond, if trisubstituted, favors E, whereas the major conformation of the nascent intermediate, aminocrotonate, is z (defined as relative to the amino group); and (4) protonation at C-4 is mediated by a different enzyme base which is not shielded and is situated at the si face with respect to the α-C atom.

IT **91366-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with bromine and sodium hydroxide)

RN 91366-30-2 CAPLUS

CN Cyclopropane-2,2,3,3-d4-carboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1971:551666 CAPLUS

DN 75:151666

TI 5-Azaspiro[2.4]heptane-4,6-diones

IN German, Victor F.

PA A. H. Robins Co., Inc.

SO Ger. Offen., 25 pp.
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2103576	A	19710826	DE 1971-2103576	19710126
	US 3654306	A	19720404	US 1970-5904	19700126
	ES 386409	A1	19731201	ES 1970-386409	19701212
	GB 1307341	A	19730221	GB 1971-1497	19710112
	CA 942753	A1	19740226	CA 1971-103115	19710119
	ZA 7100471	A	19711124	ZA 1971-471	19710125
	FR 2081459	A1	19711203	FR 1971-2365	19710125
	FR 2081459	A5	19711203		
	CH 547798	A	19740411	CH 1971-1078	19710125
PRAI	US 1970-5904	A	19700126		

GI For diagram(s), see printed CA Issue.

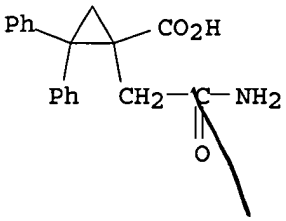
AB Title compds. (I), useful as diuretics and intermediates for antidepressant 5-azaspiro[2.4]heptanes, were prepared from MeO2CCH2C(:CH2)CO2Me (II) by reaction with diazomethanes CRPhN2 (III) to give Me α-[1-(carbomethoxy)-2-R,2-Ph-disubstituted-cyclopropyl]acetates, followed by hydrolysis and cyclization to give 1-R,1-Ph-disubstituted 5-oxaspiro[2.4]heptane-4,6-diones (IV), subsequent reaction with R1NH2, and cyclization. I were also prepared from itaconic anhydride (V) by reaction with R1NH2 to give R1NHCOCH2C(:CH2)CO2H, followed by cyclization, and reaction with III. Thus, II reacted with p-MeC6H4CPhN2 in Et2O 3 days at room temperature to give Me α-[1-(carbomethoxy)-2-phenyl-2-(p-tolyl)cyclopropyl]acetate, which was refluxed with KOH in EtOH 6 hr. The reaction product was refluxed with Ac2O to

give IV (R=p-tolyl), which was treated with urea to give I (R=p-MeC6H4, R1=H). V was treated with III (R=p-tolyl) to give 90% IV (R=p-tolyl). V was treated with PhNH2 at 5-10° in ether to give 81% 2-methylenesuccinanilide, which was treated with NaOAc and Ac2O 1 hr at 50° to give 40% N-phenyl-2-methylenesuccinimide, which was treated with CPh2N2 in ether to give 64% I (R=R1=Ph). Similarly prepared were I (R=Ph, R1 given): H, CH2Ph, Me, CH2CH2Ph, Ph, Et and I (R=p-MeOC6H4, R1=H).

IT **34105-37-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34105-37-8 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(carbamoylmethyl)-2,2-diphenyl- (8CI) (CA INDEX NAME)



L3 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1966:18555 CAPLUS

DN 64:18555

OREF 64:3322c-f

TI N.M.R. study of cyclopropane. I. Investigation of certain cyclopropane derivatives by nuclear magnetic resonance

AU Pavia, Andre Armand; Wylde, James; Wylde, Renee; Arnal, Elian

CS Ecole Natl. Super. Chim., Montpellier

SO Bulletin de la Societe Chimique de France (1965), (10), 2709-18
CODEN: BSCFAS; ISSN: 0037-8968

DT Journal

LA French

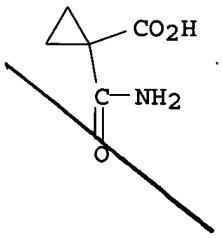
AB Relatively simple 1,1-disubstituted and 1,1,2,2-tetrasubstituted cyclopropane derivs. were prepared and studied by N.M.R. The variation of the chemical shift and the coupling consts. of the protons were studied as a function of the attracting power of the electrons of the substituents of the ring. For substituents such as CN or Ph, which exert a strong long distance effect, the anisotropy correction must be used if the measured chemical shifts are to correctly express the attracting power of these groups. Exptl. results obtained showed a very definite variation of the chemical shifts as a function of the substituent. The Taft coupling consts. were used to measure the attracting power of the substituents. The decrease of magnetic protection or deshielding by the attracting effect of the electrons was less than, but of the same order of magnitude, as that measured for unsatd. compds. This observation favors a pseudo-unsatd. structure for cyclopropane. The greater polarizability of the electronic structure can partly explain the relative ease of cyclopropane to transmit electronic effects. Math. proof is given to confirm the hypothesis that, in cyclopropane esters, the cis β protons absorb in weaker fields than the trans protons. The equation which quant. evaluates the long distance effect of the triple bond contains all the parameters determining the reciprocal position of the substituents and the parameters belonging to the involved bond: $\Delta\omega = 1/3\ \Delta\chi(3\ \cos 2\alpha - 1)R^{-3}$ where $\Delta\omega$ is the displacement in cycles/sec. to be evaluated, R is the distance between the center of the triple bond and the proton considered, α is the angle between the axis of the triple bond and the line joining the center of the triple bond and the proton considered,

and $\Delta\chi = \chi L - \chi T$ measures the magnetic susceptibility of the triple bond.

IT **6914-74-5**, Cyclopropanecarboxylic acid, 1-carbamoyl- (nuclear magnetic resonance of)

RN 6914-74-5 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(aminocarbonyl)- (9CI) (CA INDEX NAME)



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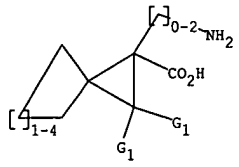

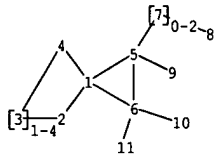

R_1 R_2 cyclic from C_4 to C_8

cyclobutane to cyclooctane

chain nodes :
7 8 9 10 11
ring nodes :
1 2 3 4 5 6
chain bonds :
5-7 5-9 6-10 6-11 7-8
ring bonds :
1-2 1-4 1-5 1-6 2-3 3-4 5-6
exact/norm bonds :
1-2 1-4 1-5 1-6 2-3 3-4 5-6 6-10 6-11 7-8
exact bonds :
5-7 5-9

G1:C,H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS

10760032-R3 AND R4 NON CICLYC

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NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 26	CA/CAPLUS - Expanded patent coverage to include the Russian Agency for Patents and Trademarks (ROSPATENT)
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

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NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

10760032-R3 AND R4 NON CICLYC

FILE 'HOME' ENTERED AT 15:15:07 ON 11 FEB 2005

=> FILE REGISTRY
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:15:27 ON 11 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 9 FEB 2005 HIGHEST RN 828241-21-0
DICTIONARY FILE UPDATES: 9 FEB 2005 HIGHEST RN 828241-21-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L1 STRUCTURE UPLOADED

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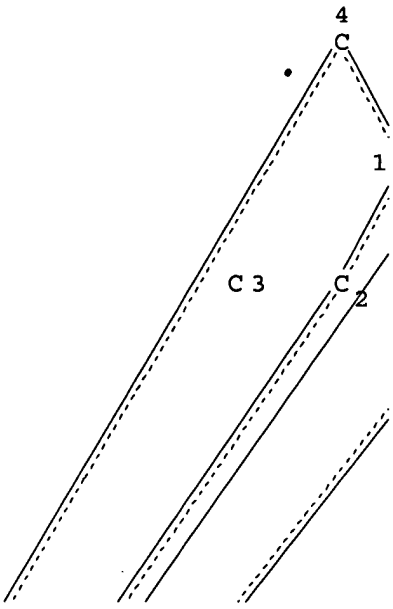
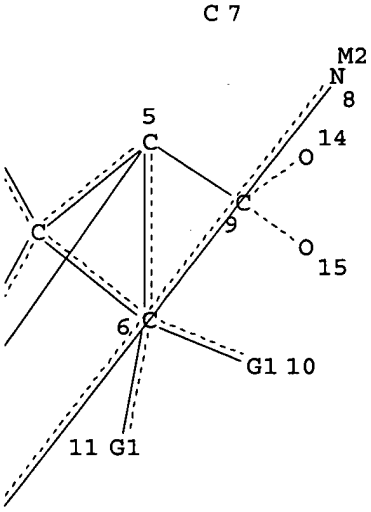
L1 HAS NO ANSWERS
L1 STR

10760032-R3 AND R4 NON CICLYC

C 16 H 18 C M3

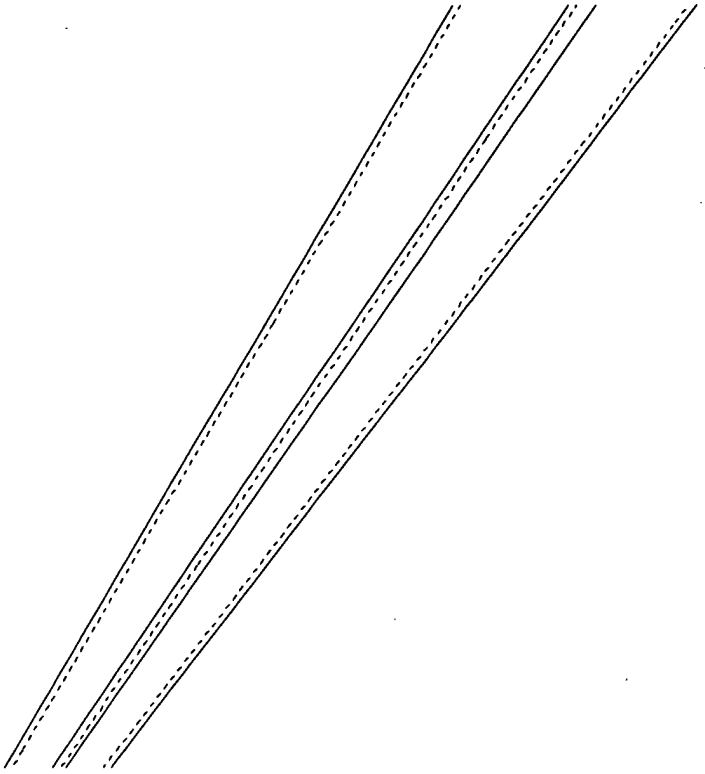


Page 1-A

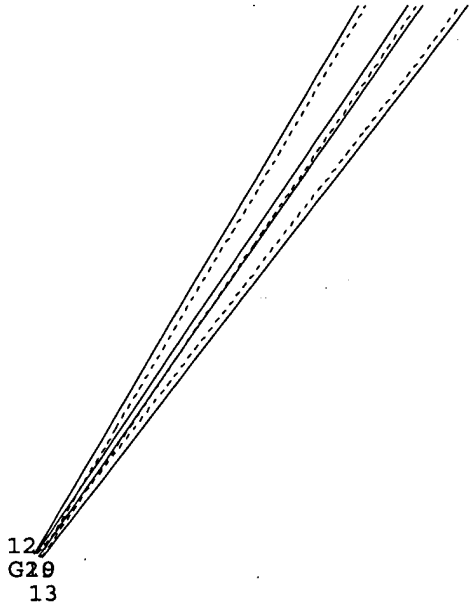


Page 1-B

10760032-R3 AND R4 NON CICLYC



Page 2-A



Page 3-A

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REP G20=(0-2) 7-5 7-8
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HCOUNT  IS M3     AT  18
NSPEC   IS R      AT   1
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10760032-R3 AND R4 NON CICLYC

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NSPEC   IS R      AT   4
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NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
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MLEVEL  IS CLASS  AT   7  8  9 14 15 16 17 18
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE


=> S L1 FULL
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FULL SCREEN SEARCH COMPLETED -    191 TO ITERATE

100.0% PROCESSED     191 ITERATIONS                          16 ANSWERS
SEARCH TIME: 00.00.01

L2            16 SEA SSS FUL L1

=> FILE CAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.76     161.97

FILE 'CAPLUS' ENTERED AT 15:16:33 ON 11 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 11 Feb 2005  VOL 142 ISS 7
FILE LAST UPDATED: 9 Feb 2005  (20050209/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
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10760032-R3 AND R4 NON CICLYC

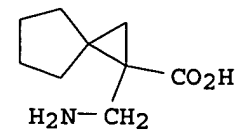
=> S L2 FULL
L3 4 L2

=> D 1-4 BIB ABS HITSTR L3

L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:756699 CAPLUS
DN 141:277627
TI Preparation of tetrazole and oxadiazolone substituted β-amino acid derivatives as ligands of the α2δ-subunit of a calcium channel
IN Barta, Nancy Sue; Colbry, Norman Lloyd; Hudack, Raymond Andrew, Jr.; Lin, Kristin Knapp; Schwarz, Jacob Bradley; Thorpe, Andrew John; Wustrow, David Juergen; Zhu, Zhijian
PA Warner-Lambert Company LLC, USA
SO PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004078734	A1	20040916	WO 2004-IB510	20040223
	W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2005014804	A1	20050120	US 2004-795760	20040308
PRAI	US 2003-452871P	P	20030307		

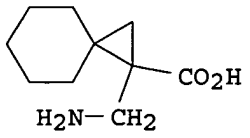
OS MARPAT 141:277627
AB Title compds. R2R1(NH2)C-C(G)R3R4 [G = tetrazolyl, 1,3,5-oxadiazol-2-one; R1-2 = H, alkyl, alkoxy, etc.; R3-4 = H, Me; (I)] and related cyclopropane derivs. are prepared For instance, 4-methyl-2-(1H-tetrazol-5-yl)pentylamine is prepared from 1-benzyl-1H-tetrazole and 4-methyl-1-nitropentene in 2 steps. Selected example compds. exhibit binding with nM to μM affinity for α2δ-subunit of the calcium channel (3 biol. examples). I are useful for the treatment of central nervous system and other disorders.
IT **724772-88-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tetrazole and oxadiazolone substituted β-amino acid derivs. as ligands of α2δ-subunit of a calcium channel for use as CNS agents)
RN 724772-88-7 CAPLUS
CN Spiro[2.4]heptane-1-carboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



NO Prior art

10760032-R3 AND R4 NON CICLYC

IT **724773-58-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrazole and oxadiazolone substituted β-amino acid derivs. as ligands of α2δ-subunit of a calcium channel for use as CNS agents)
RN 724773-58-4 CAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-(aminomethyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

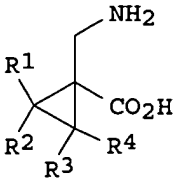
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:612495 CAPLUS
DN 141:123903
TI Preparation of cyclopropyl β-amino acid derivatives for pharmaceutical use
IN Schwarz, Jacob Bradley; Wustrow, David Juergen
PA USA
SO U.S. Pat. Appl. Publ., 22 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004147608	A1	20040729	US 2004-760032	20040116
	WO 2004065361	A2	20040805	WO 2004-IB58	20040109
	WO 2004065361	A3	20041007		

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI

PRAI US 2003-441825P P 20030122
OS MARPAT 141:123903
GI



I

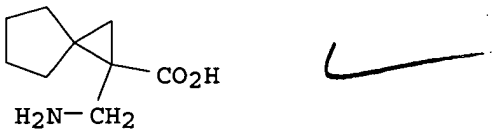
10760032-R3 AND R4 NON CICLYC

AB The invention relates to novel cyclopropyl β-amino acids derivs. I [R1 and R2 are H, alkyl, alkoxyalkyl, phenylalkyl or phenylalkoxyalkyl, where the Ph moieties can optionally be substituted with one or two halo or alkyl groups; or R1R2C is cyclopentyl, cyclohexyl or cycloheptyl which can be substituted with one or two groups R1/R2; R3, R4 are H or Me] and pharmaceutical compns. containing them for use in the treatment of central nervous system and other disorders. Compds. I exhibit activity as α2δ ligands and have affinity for the α2δ subunit of a calcium channel. Thus, 1-aminomethylspiro[2.5]octane-1-carboxylic acid hydrochloride was prepared by treating cyanocyclohexylideneacetic acid Et ester with nitromethane in MeCN in the presence of DBU, followed by hydrogenation over Raney Ni and hydrolysis with 3N HCl.

IT **724772-88-7P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopropyl β-amino acid derivs. for pharmaceutical use)

RN 724772-88-7 CAPLUS

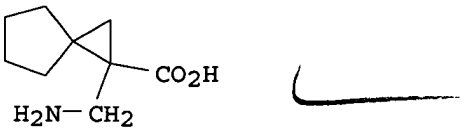
CN Spiro[2.4]heptane-1-carboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



IT **724772-85-4P 724772-86-5P 724772-87-6P**
724772-92-3P 724772-97-8P 724772-98-9P
724773-02-8P 724773-04-0P 724773-05-1P
724773-06-2P 724773-07-3P 724773-58-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopropyl β-amino acid derivs. for pharmaceutical use)

RN 724772-85-4 CAPLUS

CN Spiro[2.4]heptane-1-carboxylic acid, 1-(aminomethyl)-, hydrochloride (9CI) (CA INDEX NAME)

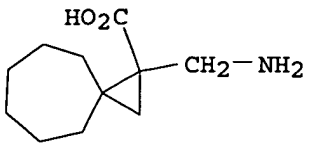


● HCl

RN 724772-86-5 CAPLUS

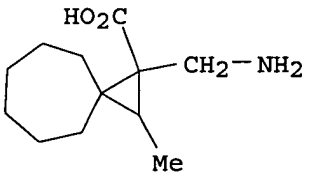
CN Spiro[2.6]nonane-1-carboxylic acid, 1-(aminomethyl)-, hydrochloride (9CI) (CA INDEX NAME)

10760032-R3 AND R4 NON CICLYC

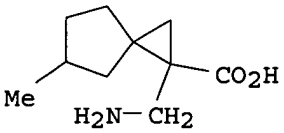


● HCl

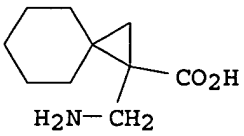
RN 724772-87-6 CAPLUS
CN Spiro[2.6]nonane-1-carboxylic acid, 1-(aminomethyl)-2-methyl- (9CI) (CA INDEX NAME)



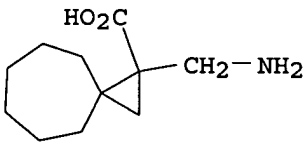
RN 724772-92-3 CAPLUS
CN Spiro[2.4]heptane-1-carboxylic acid, 1-(aminomethyl)-5-methyl- (9CI) (CA INDEX NAME)



RN 724772-97-8 CAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



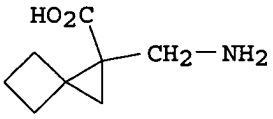
RN 724772-98-9 CAPLUS
CN Spiro[2.6]nonane-1-carboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



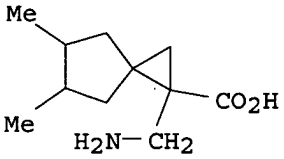
RN 724773-02-8 CAPLUS

10760032-R3 AND R4 NON CICLYC

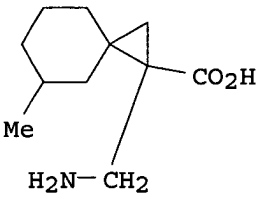
CN Spiro[2.3]hexane-1-carboxylic acid, 1-(aminomethyl)- (9CI) (CA INDEX NAME)



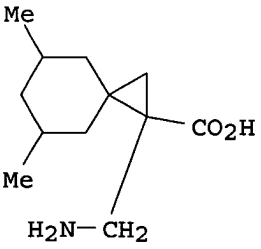
RN 724773-04-0 CAPLUS
CN Spiro[2.4]heptane-1-carboxylic acid, 1-(aminomethyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



RN 724773-05-1 CAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-(aminomethyl)-5-methyl- (9CI) (CA INDEX NAME)

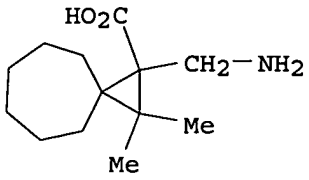


RN 724773-06-2 CAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-(aminomethyl)-5,7-dimethyl- (9CI) (CA INDEX NAME)

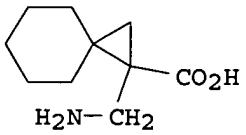


RN 724773-07-3 CAPLUS
CN Spiro[2.6]nonane-1-carboxylic acid, 1-(aminomethyl)-2,2-dimethyl- (9CI) (CA INDEX NAME)

10760032-R3 AND R4 NON CICLYC



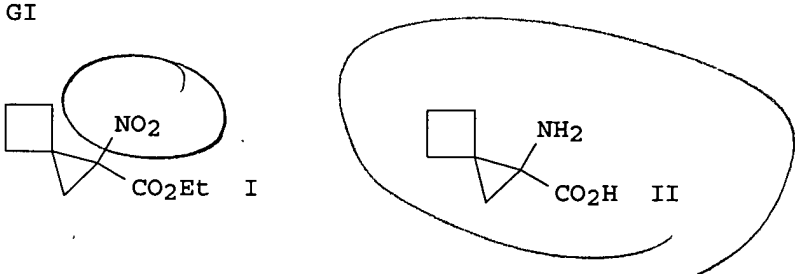
RN 724773-58-4 CAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-(aminomethyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L3 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:807840 CAPLUS
DN 139:396150
TI Catalytic cyclopropanation of methylenecyclobutanes using ethyl nitrodiazoacetate. Synthesis of spirohexane amino acids
AU Yashin, Nikolai V.; Averina, Elena B.; Gerdov, Sergei M.; Kuznetsova, Tamara S.; Zefirov, Nikolai S.
CS Department of Chemistry, Moscow State University, Moscow, 119899, Russia
SO Tetrahedron Letters (2003), 44(45), 8241-8244
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 139:396150
GI

check Date in library 2003

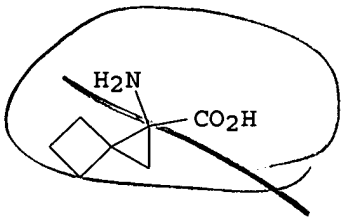


AB The reaction of Et nitrodiazoacetate with a series of methylenecyclobutanes was studied and both [1+2]- and [2+3]-cycloaddn. pathways were observed depending on olefin structure. Amino acids of a spirohexane type were synthesized from methylenecyclobutanes by a three-step synthesis. For example, methylenecyclobutane reacted with Et nitrodiazoacetate in presence of Rh2(OAc)4 in CH2Cl2 at room temperature to give nitro derivative I in 89% yield, which was converted to amino acid II in two steps (treatment with HCO2NH4; Pd/C in MeOH at room temperature) with 56% yield.

IT **625827-37-4P 625827-39-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of spirohexane amino acids via catalytic cyclopropanation of

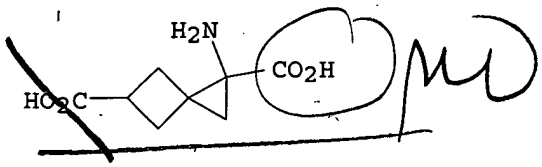
10760032-R3 AND R4 NON CICLYC

methylenecyclobutanes with nitrodiazoacetate)
RN 625827-37-4 CAPLUS
CN Spiro[2.3]hexane-1-carboxylic acid, 1-amino- (9CI) (CA INDEX NAME)



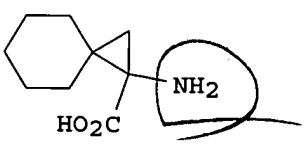
a "CH_2" less in the ring and another one in NH_2 more!

RN 625827-39-6 CAPLUS
CN Spiro[2.3]hexane-1,5-dicarboxylic acid, 1-amino- (9CI) (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:231440 CAPLUS
DN 122:10523
TI Straightforward Synthesis of 1-Amino-2,2-dialkylcyclopropanecarboxylic Acids via Selective Saponification of 2,2-Dialkylcyclopropane-1,1-dicarboxylic Esters and Curtius Rearrangement
AU De Kimpe, Norbert; Boeykens, Marc; Tehrani, Kourosch Abbaspour
CS Faculty of Agricultural and Applied Biological Sciences, University of Gent, Ghent, B-9000, Belg.
SO Journal of Organic Chemistry (1994), 59(26), 8215-19
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 122:10523
AB Selective monosaponification of di-Me 2,2-dialkylcyclopropane-1,1-dicarboxylic esters afforded the corresponding 2,2-dialkyl-1-(methoxycarbonyl)cyclopropane-1-carboxylic acids, which were rearranged with di-Ph phosphoroazidate via a modified Curtius-type reaction to give Me 2,2-dialkyl-1-(N-(alkoxycarbonyl)amino)cyclopropanecarboxylic esters. Selective deprotection of the carbamate or Me cyclopropanecarboxylic ester was worked out, giving rise to a whole variety of aminocyclopropanecarboxylate analogs.
IT **159279-82-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(straightforward synthesis of amino(dialkyl)cyclopropanecarboxylic acids via selective saponification of diesters and Curtius rearrangement)
RN 159279-82-0 CAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-amino- (9CI) (CA INDEX NAME)



103 a "CH_2" less

further

10760032-R3 AND R4 NON CICLYC